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Statistical foundations of liquid-crystal theory:

II: Macroscopic balance laws

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Abstract

Working on a state space determined by considering a discrete system of rigid rods, we use nonequilibrium statistical mechanics to derive macroscopic balance laws for liquid crystals. A probability function that satisfies the Liouville equation serves as the starting point for deriving each macroscopic balance. The terms appearing in the derived balances are interpreted as expected values and explicit formulas for these terms are obtained. Among the list of derived balances appear two, the tensor moment of inertia balance and the mesofluctuation balance, that are not standard in previously proposed macroscopic theories for liquid crystals but which have precedents in other theories for structured media.

Keywords

Statistical mechanics; discrete-to-continuum limit; balance laws; fluctuations; Reynolds stress

1 Introduction

In the present paper, we adapt Noll's [1] extension of the approach of Irving & Kirkwood [2] to derive macroscopic balance laws for a theory of liquid crystals in which the microstructure is described by a symmetric and traceless tensor. In so doing, our objective is to provide perspective regarding the microphysical basis of the balances and the various terms that enter them. Challenges related to formulating constitutive equations and boundary conditions, which would be necessary to state and analyze initial-boundary-value problems, are therefore not addressed.

Irving & Kirkwood [2] considered a system comprised by a finite number of identical particles. A state of this system consists of the collection of positions and velocities of each of the constituent particles. Forces between the particles are assumed to derive from a potential. The likelihood of finding the system in a given state is determined by a probability function that satisfies the Liouville equation. This evolution equation provides the basis for deriving all balance laws. The terms appearing in these laws are given by explicit formulas.

In contrast to Irving & Kirkwood [2], Noll [1] considered systems of disparate particles, avoided reliance on the Dirac delta distribution, provided conditions sufficient to ensure that certain improper integrals converge, and interpreted the terms entering the balances as expected values.

To derive the macroscopic balance laws for conventional continua, Irving & Kirkwood [2] required the momentum balance for each particle and an interaction potentials that determine the forces exerted between particles. For liquid crystals consisting of rod-like molecules, the force balance, torque balance, and constitutive information in terms of interaction for each particle is also required. The discrete framework upon which our derivations are based appears in Part I of this paper.

Precedents for the present work are provided by Dahler & Scriven [3], Pitteri [4], and Svendsen [5]. Dahler & Scriven [3] applied the approach of Irving & Kirkwood [2] to systems of particles with unspecified internal degrees of freedom and internal angular momentum. They also allowed for non-central interactions between particles. These generalizations yield a nonstandard moment of momentum balance, similar in structure to that arising in the theory of liquid crystals. Since Dahler & Scriven [3] did not impose any particular structure for the particles, a direct comparison of the macroscopic balance laws they obtain and those governing liquid crystals is problematic. Pitteri [4] considered a discrete system consisting of subsystems of particles that are constrained to represent molecules. Using the methods of Irving & Kirkwood [2] and Noll [1], Pitteri derived the macroscopic balance of energy. He then employed the approach of Green & Rivlin [6], which assumes that the energy balance is invariant under superposed rigid motions, to obtain the balances for mass, momentum, moment of momentum, and tensor moment of inertia. Pitteri [4] did not obtain an analog of the orientation balance of liquid-crystal theory. Indeed, to our knowledge, the literature does not currently contain an invariance-based argument that yields the orientation balance of liquid-crystal theory. Pitteri gave statistical formulas for all of the terms appearing in his balances but did not justify these formulas as Noll [1] did. Svendsen [5] considered a collection of particles governed by interactions that in addition to conventional conservative forces may also include dissipative forces. Svendsen [5] derived discrete balances for higher-order velocity moments. These precursors to the macroscopic balances, one of which is the momentum flux balance, the trace of which gives the energy balance. Using the approach of Irving & Kirkwood [2] and Noll [1], Svendsen [5] obtained macroscopic balances for mass, tensor moment of inertia, momentum, moment of momentum, and energy. Like Pitteri [4], Svendsen [5] gave statistical formulas for all of the terms appearing in his balances but did not justify these formulas.

The approach of Irving & Kirkwood [2] should not be confused with that used in the kinetic theory of gases (see, for example, Chapman & Cowling [7], Truesdell & Muncaster [8], and Cercignani [9]). One fundamental difference between these approaches is that in the kinetic theory particle interactions are governed not by forces but rather by collisions, as described by a collision operator. Moreover, in the kinetic theory, macroscopic quantities are obtained by computing moments of a phase-space density governed by the Maxwell–Boltzmann equation. In general, the procedure generates an infinite hierarchy of evolution equations. The evolution equation for any moment generally involves the next highest moment. Thus,

truncating the kinetic equations at any moment does not provide a closed description unless additional information relating the next highest moment to the lower moments is introduced. In contrast, the approach of Irving & Kirkwood [2] and Noll [1] yields macroscopic balance laws that involve fields, such as the Cauchy stress, that embody internal interactions and a closed description rests on the provision of additional constitutive laws for those fields.

The approach of Irving & Kirkwood [2] should also not be confused with that taken in work focused on using statistical mechanics to derive macroscopic free-energy densities. For liquid crystals, a comprehensive description of this approach, including discussion of the seminal contributions of Grandjean [10], Onsager [11], and Maier & Saupe [12], is given by Jákli & Saupe [13]. Building on such equilibrium theories, Hess [14], Doi & Edwards [15, 16, 17], and Marucci & Greco [18] developed kinetic theories for suspensions of rod-like molecules in which a rotary phase-space density (or orientation distribution function) is governed by a Fokker–Plank equation. For detailed reviews of the associated literature, see Chan & Terentjev [19] and Kröger [20]. For descriptions and comparisons of various closure schemes, see Feng, Chaubal & Leal [21] and Kröger [20].

Although most theories of liquid crystals are based on the assumption that the underlying molecules possess an axis of rotational symmetry, the implications of relaxing this assumption have been explored. Straley [22] put forward a theory in which the molecules are modeled by rectangular prisms elongated in one direction. To describe a liquid crystal consisting of such molecules, four scalar order parameters are needed: two describe the distribution of the direction associated with the long axis and two more to describe the distribution of the direction of the short axes. It is possible to describe these four order parameters by two traceless symmetric second-order tensors, one of which being analogous to that used by MacMillan [23], as explained by Sonnet, Virga, & Durand [24]. Straley [22] obtained orientation balance laws for his order parameters by averaging the orientations of the molecules weighted with a probability distribution when the molecules are governed by an interaction energy. While Straley [22] obtained an orientation balance, he did not justify the terms that appear in his balances.

There have been other justifications of the macroscopic balances for liquid crystals, some of which are not based on statistical methods. For example, Blenk & Muschik [25] derived the macroscopic balances for liquid crystals using a completely different approach. They considered a liquid crystal to be a mixture of different fluids, each fluid having a constant, but distinct, orientation. They wrote down the balances for each component of the mixture and then averaged these balances over all of the components in the mixture to obtain the balance laws for the mixture.

Connections between various features of the discrete and continuous descriptions of liquid crystals can be found in the literature. Lubensky [26] contributed a precise formula for the director in terms of the orientations of the constituent molecules. This was achieved by first modeling the molecules as rigid rods with orientations described by unit vectors. These unit vectors were then used to form a tensor order parameter that is symmetric and traceless and measures how far the state of the medium deviates from isotropic—that is, from a state in which the rods are randomly oriented. Importantly, it transpires that the unit vector

associated with the largest eigenvalue of the tensor order parameter corresponds to the order parameter used in the director theories. Although Lubensky [26] determined an expression for the additional inertial contribution to the moment of momentum balance, he gave no formulas for the additional terms appearing in the moment of momentum and energy balances. In contrast to the theories of Oseen [27] and Ericksen [28], which include an additional balance law for the order parameter, Lubensky [26] introduced a supplemental compatibility condition and used it to derive the additional balance law from the moment of momentum balance. This condition relates the couple-stress tensor and the Cauchy stress to the noninertial terms that appear in the evolution equation for the vector order-parameter. On the basis of this compatibility condition, Lubensky [26] argued that the evolution equation for the order parameter is a consequence of the moment of momentum balance.

Beginning with a careful inspection of the moment of momentum balance for a single rigid rod, Müller [29] furnished some motivation for the additional terms in the macroscopic moment of momentum balance for a liquid crystal. Recognizing that the configuration of a rigid rod is completely determined by the position of its center of mass and a unit vector describing its orientation, Müller [29] decomposed each term in the moment of momentum balance into components associated with the center of mass and orientation of the rod. He then used these terms for guidance in formulating a macroscopic balance for the moment of momentum. In a similar fashion, Müller [29] motivated the additional terms in the energy balance. Like Lubensky [26], Müller [29] stipulated a compatibility condition which, in combination with the moment of momentum balance, yields an evolution equation for the order parameter.

The orientation balance merits additional discussion. As mentioned above, there are two distinct approaches to arriving at an equation governing the evolution of the order parameter. Whereas some workers postulate it independent of the other balance laws, others derive it from the moment of momentum balance under the presumption that a compatibility condition holds. These approaches both carry elements of truth. When considering systems of rigid rods, we derive a balance from the moment of momentum balance that can be viewed as a microscopic precursor of the orientation balance. However, when obtaining the macroscopic balance laws for liquid crystals via statistics, the orientation balance arises from considerations independent of those used to arrive at other balances. An analogous development is tied to the moment of momentum balance in classical particle mechanics. In that setting, granted that particle-particle interactions are governed by a potential depending only on the distance between the particles and the orientation of the line connecting the particles, the forces between particles are equal and opposite and are directed along the line connecting the particles. Using this, the moment of momentum balance for systems of particles can be derived from the momentum balance. Nevertheless, the macroscopic moment of momentum balance ensues using statistics independent of those leading to the macroscopic momentum balance.

The continuum balance laws for liquid crystals that we derive resemble those of Ericksen [28] and MacMillan [23], with some important differences. One of these lies with the orientation balance. Our version of that balance contains two new terms. One of these we identify as a Reynolds tensor, and the other describes the relative average rate of the

orientation tensor. These quantities are kinematical in nature and thus are not specified by constitutive laws. Additional balance laws are needed to describe the evolution of these additional quantities.

Precedents for these additional ingredients appear in the works Pitteri [4] and Capriz [30]. Pitteri [4] obtained a balance for the tensor moment of inertia. Inspection of the expression determining that tensor shows that the balance in which it appears is equivalent to the balance we obtain for the relative average rate of the orientation tensor. The Reynolds tensor is of importance in the theory for ephemeral continua introduced by Capriz [30] and developed further by Brocato & Capriz [31]. The primary feature that distinguishes an ephemeral continuum from a conventional continuum rests in the nature of material points. In the theory of ephemeral continua, each material point consists of a collection of subpoints, intended to represent molecules, that can migrate between material points. The subpoints comprising a material point can be in different states, as described by a position within the material point and a velocity. By performing weighted averages of various microscopic quantities associated with each molecule, such as their momentum, over the set of all states, Capriz obtained formulas for several macroscopic quantities of importance. He then wrote down balances involving these quantities. Whereas Capriz [30] did not attempt to derive these balance laws, Brocato & Capriz [31] used an extended kinetic theory to do so. One term that possesses a statistical formula is the Reynolds tensor, which appears in the symmetric part of the tensor moment of momentum balance. This term is governed by a non-standard tensor balance law, called the mesofluctuation balance. Inasmuch as its terms carry dimensions of energy per unit volume per unit time, this balance has the flavor of a tensor energy balance. Importantly, however, the trace of the mesofluctuation balance does not coincide with the traditional scalar energy balance. Since the terms appearing in the mesofluctuation balance have similar statistical formulas to those appearing in the balance that we obtain for the Reynolds tensor, we refer to it as a mesofluctuation balance.

The paper is laid out as follows. The probability density, which is essential to the statistical argument, is introduced in Section 2. The macroscopic balance laws for liquid crystals and the statistical formulas for the macroscopic state functions appearing in these laws are set down in Section 3. Justifications of these formulas are provided in Section 4. Detailed derivations of balances appear in Section 5. Our most important results are summarized in Section 6.

2 The probability density

Let $\mathcal{B}$ be a system of rigid rods. As can be seen from the previous section, the *state* of a rod p in $\mathcal{B}$ is determined by the position of its center, its director, and the rate of change of both of these—that is, a quadruple $(x_p, \mathbf{v}_p, \mathbf{d}_p, \mathbf{s}_p)$ belonging to

$$\mathcal{E} \times \mathcal{V} \times \mathcal{U}_\perp^2. \quad (1)$$

The states of the system $\mathcal{B}$ therefore consist of a quadruple $(x_p, \mathbf{v}_p, \mathbf{d}_p, \mathbf{s}_p)$ for all rods p in $\mathcal{B}$ and will denote the set of all states by Ω , which we refer to as the phase space. Furthermore, we will denote an element of Ω by

$$((x_p, \mathbf{v}_p, \mathbf{d}_p, \mathbf{s}_p) | p \in \mathcal{B}). \quad (2)$$

If the state of the system is known, then the microscopic constitutive relations of Seguin & Fried [32] determine the forces and torques acting on the system. We assume there is a C^1 function

$$W: \Omega \times \mathcal{I} \rightarrow \mathbb{P} \quad (3)$$

that gives the probability density of the states in Ω at each time. Using the fact that W is defined on a manifold on which $\mathbf{d}_p \cdot \mathbf{s}_p = 0$, one may show that the vector $\nabla_{\mathbf{s}_p} W$ is perpendicular to $\mathbf{d}_p$ —that is,

$$\nabla_{\mathbf{s}_p} W = \mathbf{P}_p \nabla_{\mathbf{s}_p} W, \quad (4)$$

where $\mathbf{P}_p := \mathbf{1}_p - \mathbf{d}_p \otimes \mathbf{d}_p$ is the projection onto the plane perpendicular to $\mathbf{d}_p$.

Following Irving & Kirkwood [2] and Noll [1], we rely on a principle of conservation of probability, whereby the probability density satisfies a Liouville equation of the form

$$0 = W' + \sum_{p \in \mathcal{B}} (\nabla_{x_p} W \cdot \mathbf{v}_p + \text{div}_{\mathbf{v}_p} (W \dot{\mathbf{v}}_p) + \nabla_{\mathbf{d}_p} W \cdot \mathbf{s}_p + \text{div}_{\mathbf{s}_p} (W \mathbf{P}_p \dot{\mathbf{s}}_p)), \quad (5)$$

where W' denotes the partial derivative of W with respect to time. To eliminate the acceleration $\dot{\mathbf{v}}_p$ and rate of spin $\dot{\mathbf{s}}_p$ of rod p from the summand of (5), we use the constitutively augmented microscopic momentum and moment of momentum balances, (169) and (170), for rod p of Seguin & Fried [32], which have the respective forms

$$-\nabla_{x_p} \psi + \mathbf{f}_p^{\text{ni}} = m \dot{\mathbf{v}}_p \quad (6)$$

and

$$-\nabla_{\mathbf{d}_p} \psi + \mathbf{c}_p^{\text{ni}} = I \dot{\mathbf{s}}_p + (\lambda_p - \sum_{q \in \mathcal{B}_p} \lambda_{pq}) \mathbf{d}_p, \quad (7)$$

to give

$$0=W'+\sum_{q\in\mathcal{B}}\left[\nabla_{x_q}W\cdot\mathbf{v}_q+\frac{1}{m}\operatorname{div}_{\mathbf{v}_q}\left(W(-\nabla_{x_q}\psi+\mathbf{f}_q^{\text{ni}})\right)+\nabla_{\mathbf{d}_q}W\cdot\mathbf{s}_q+\frac{1}{I}\operatorname{div}_{\mathbf{s}_q}\left(W\mathbf{P}_q(-\nabla_{\mathbf{d}_q}\psi+\mathbf{c}_q^{\text{ni}})\right)\right].$$

$$(8)$$

Recall, from Seguin & Fried [32], that ψ is defined such that

$$\nabla_{x_p}\psi=-\sum_{q\in\mathcal{B}_p}\mathbf{f}_{pq}, \quad (9)$$

$$\nabla_{\mathbf{d}_p}\psi=-\sum_{q\in\mathcal{B}_p}(\mathbf{c}_{pq}-\lambda_{pq}\mathbf{d}_p). \quad (10)$$

3 Synopsis of central results

Here we present our main results. The macroscopic balance laws that arise from adapting Noll's [1] extension of the approach of Irving & Kirkwood [2] are listed in Subsection 3.1. Statistical formulas for the terms that appear in the macroscopic balance laws are stated in Subsection 3.2. Sufficient conditions for the convergence of the integrals that appear in the statistical formulas are given in Subsection 3.3. Finally, discussion of the macroscopic balance laws and their relation to those previously proposed for liquid crystals is contained in Subsection 3.4.

3.1 Macroscopic balance laws

We derive in Section 5 the following balances:

- Mass balance

$$\dot{\rho}+\rho\operatorname{div}\mathbf{v}=0. \quad (11)$$

- Tensor moment of inertia balance

$$\rho\Delta+\operatorname{div}\Pi=\mathbf{0}$$

(12)

- Momentum balance

$$\rho\dot{\mathbf{v}}=\operatorname{div}\mathbf{T}+\rho\mathbf{b}. \quad (13)$$

- Moment of momentum balance

$$\rho\sigma\dot{\mathbf{S}} = \frac{1}{\sqrt{2}}(\mathbf{T}^\top - \mathbf{T}) + \text{div } \mathbb{C} + \rho\mathbf{B} \quad (14)$$

- Orientation balance

$$\rho\sigma(\ddot{\boldsymbol{\Theta}} + \dot{\boldsymbol{\Delta}} - \mathbf{H}) = \mathbf{N} + \text{div } \mathbb{L} + \rho\mathbf{M}. \quad (15)$$

- Mesofluctuation balance

$$\rho\sigma\dot{\mathbf{H}} = \mathbf{Z} + \text{div } \mathbb{G} + \rho\mathbf{J}. \quad (16)$$

- Energy balance

$$\dot{e} + e \text{ div } \mathbf{v} + \text{div}(\mathbf{q} - \mathbf{T}^\top \mathbf{v} - \mathbb{L}^\top (\dot{\boldsymbol{\Theta}} + \boldsymbol{\Delta})) = \rho \mathbf{b} \cdot \mathbf{v} + \rho \mathbf{M} \cdot (\dot{\boldsymbol{\Theta}} + \boldsymbol{\Delta}) + r. \quad (17)$$

The superposed dot appearing in (11) and (13)–(17) signifies the material time-derivative and

$$\sigma = \frac{I}{m} \quad (18)$$

denotes the moment of inertia, per unit mass, of a microscopic rod. These balances relate state functions which are mappings of position and time. Of these state functions, some,

ρ = mass density,
 $\mathbf{v}$ = velocity,
 $\mathbf{S}$ = spin,
 $\mathbf{T}$ = stress tensor,
 $\mathbb{C}$ = couple tensor,
 $\mathbf{b}$ = noninertial body force per unit mass,
 $\mathbf{B}$ = noninertial body-couple per unit mass,
 e = energy density,
 $\mathbf{q}$ = heat flux,
 r = radiation,

are present in theories of Cosserat [33] continua, while others

$\boldsymbol{\Theta}$ = orientation tensor,

Π = orientation flux tensor,
 = relative average rate,
 $\mathbf{H}$ = Reynolds tensor,
 $\mathbb{L}$ = orientation-couple tensor,
 $\mathbb{G}$ = power flux tensor,
 $\mathbf{N}$ = internal orientation-couple density,
 $\mathbf{Z}$ = internal mesofluctuation density,
 $\mathbf{M}$ = noninertial orientation-couple density,
 $\mathbf{J}$ = noninertial body-mesofluctuation per unit mass,

are more exotic.

3.2 State functions as expected values

The above balance laws are subsequently derived subject to the provision that the state functions can be interpreted as expected values. To convey these expected values, it is convenient to introduce some notation. The number of rods in the system $\mathcal{B}$ is denoted by N . The $(10N - 3)$ -dimensional manifold obtained from $\mathcal{Q}$ by discarding the space that represents the possible positions of rod p is denoted by $\mathcal{Q}_p$. Similarly, the $(10N - 6)$ -dimensional manifold obtained from $\mathcal{Q}$ by discarding the spaces that represent the possible positions of rods p and q is denoted by $\mathcal{Q}_{pq}$. Let $\mathbf{g} : \mathcal{Q} \rightarrow \mathcal{W}$ be a vector-valued mapping on the phase space. The abbreviations

$$\langle \mathbf{g} \mid x_p = x \rangle \quad \text{and} \quad \langle \mathbf{g} \mid x_p = x, x_q = \tilde{x} \rangle \quad (19)$$

denote, respectively, the integral of $\mathbf{g}$ over $\mathcal{Q}_p$, after which the position of rod p is set to x , and the integral of $\mathbf{g}$ over $\mathcal{Q}_{pq}$, after which the positions of rod p is set to x and the position of rod q is set to $\tilde{x}$. Using these abbreviations, we have the relation

$$\int_{\mathcal{E}} \langle \mathbf{g} \mid x_p = x, x_q = \tilde{x} \rangle d\tilde{x} = \langle \mathbf{g} \mid x_p = x \rangle. \quad (20)$$

In Section 4, it is shown that the expected values of the state functions are given as delineated below.

The mass density ρ , velocity $\mathbf{v}$, orientation tensor $\mathbf{\Theta}$, and orientation flux tensor Π are given by

$$\rho = \sum_{p \in \mathcal{B}} \langle mW \mid x_p = x \rangle, \quad (21)$$

$$\rho \mathbf{v} = \sum_{p \in \mathcal{B}} \langle m v_p W \mid x_p = x \rangle, \quad (22)$$

$$\rho \mathbf{\Theta} = \sum_{p \in \mathcal{B}} \langle \frac{1}{2} m \mathbf{d}_p \odot \mathbf{d}_p W \mid x_p = x \rangle - \frac{\rho}{3\sqrt{2}} \mathbf{1}, \quad (23)$$

$$\mathbb{\Pi} = - \sum_{p \in \mathcal{B}} \langle m (\frac{1}{2} \mathbf{d}_p \odot \mathbf{d}_p - \mathbf{\Theta}) \otimes (\mathbf{v}_p - \mathbf{v}) W \mid x_p = x \rangle. \quad (24)$$

The spin $\mathbf{S}$, relative average rate $\mathbf{\dot{\Theta}}$, and Reynolds tensor $\mathbf{H}$ are given by

$$\rho \mathbf{S} = \sum_{p \in \mathcal{B}} \langle m \mathbf{d}_p \wedge \mathbf{s}_p W \mid x_p = x \rangle, \quad (25)$$

$$\rho \mathbf{\Delta} = \sum_{p \in \mathcal{B}} \langle m \mathbf{d}_p \odot \mathbf{s}_p W \mid x_p = x \rangle - \rho \mathbf{\dot{\Theta}}, \quad (26)$$

$$\rho \mathbf{H} = \sum_{p \in \mathcal{B}} \langle m \mathbf{s}_p \odot \mathbf{s}_p W \mid x_p = x \rangle. \quad (27)$$

The stress tensor $\mathbf{T}$ is given by the sum

$$\mathbf{T} = \mathbf{T}_k + \mathbf{T}_I \quad (28)$$

of a kinetic contribution $\mathbf{T}_K$ and an interaction contribution $\mathbf{T}_I$, with

$$\mathbf{T}_K = - \sum_{p \in \mathcal{B}} \langle m (\mathbf{v}_p - \mathbf{v}) \otimes (\mathbf{v}_p - \mathbf{v}) W \mid x_p = x \rangle, \quad (29)$$

$$\mathbf{T}_I = - \frac{1}{2} \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_{\mathcal{V}} \int_0^\infty \langle \mathbf{f}_{pq} W \mid x_p = x + \alpha \mathbf{z}, x_q = x - (1 - \alpha) \mathbf{z} \rangle \otimes \mathbf{z} \, d\alpha \, d\mathbf{z}. \quad (30)$$

The couple tensor $\mathbb{C}$ is given by the sum

$$\mathbb{C} = \mathbb{C}_K + \mathbb{C}_{IF} + \mathbb{C}_{IC} \quad (31)$$

of a kinetic contribution $\mathbb{C}_K$ and two interaction contributions, one coming from resultant forces $\mathbb{C}_{IF}$ and the other coming from resultant couples $\mathbb{C}_{IC}$, with

$$\mathbb{C}_K = - \sum_{p \in \mathcal{B}} \langle I(\mathbf{d}_p \wedge \mathbf{s}_p - \mathbf{S}) \otimes (\mathbf{v}_p - \mathbf{v}) W \mid x_p = x \rangle, \quad (32)$$

$$\mathbb{C}_{IF} = - \frac{1}{2} \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_{\mathcal{V}} \int_0^\infty \langle \alpha \mathbf{z} \wedge \mathbf{f}_{pq} W \mid x_p = x + \alpha \mathbf{z}, x_q = x - (1 - \alpha) \mathbf{z} \rangle \otimes \mathbf{z} d\alpha d\mathbf{z}, \quad (33)$$

$$\mathbb{C}_{IC} = - \frac{1}{2} \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_{\mathcal{V}} \int_0^\infty \langle \mathbf{d}_p \wedge \mathbf{c}_{pq} W \mid x_p = x + \alpha \mathbf{z}, x_q = x - (1 - \alpha) \mathbf{z} \rangle \otimes \mathbf{z} d\alpha d\mathbf{z}. \quad (34)$$

The orientation couple tensor $\mathbb{L}$ is given by the sum

$$\mathbb{L} = \mathbb{L}_K + \mathbb{L}_I \quad (35)$$

of a kinetic contribution $\mathbb{L}_K$ and an interaction contribution $\mathbb{L}_I$, with

$$\mathbb{L}_K = - \sum_{p \in \mathcal{B}} \langle I(\mathbf{d}_p \odot \mathbf{s}_p - (\dot{\mathbf{\Theta}} + \mathbf{\Delta})) \otimes (\mathbf{v}_p - \mathbf{v}) W \mid x_p = x \rangle, \quad (36)$$

$$\mathbb{L}_I = - \frac{1}{2} \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_{\mathcal{V}} \int_0^\infty \langle \mathbf{d}_p \odot \mathbf{P}_p \mathbf{c}_{pq} W \mid x_p = x + \alpha \mathbf{z}, x_q = x - (1 - \alpha) \mathbf{z} \rangle \otimes \mathbf{z} d\alpha d\mathbf{z}. \quad (37)$$

The power-flux tensor $\mathbb{G}$ is given by the sum

$$\mathbb{G} = \mathbb{G}_K + \mathbb{G}_I, \quad (38)$$

of a kinetic contribution $\mathbb{G}_K$ and an interaction contribution $\mathbb{G}_I$, with

$$\mathbb{G}_K = - \sum_{p \in \mathcal{B}} \langle I(\mathbf{s}_p \odot \mathbf{s}_p - \mathbf{H}) \otimes (\mathbf{v}_p - \mathbf{v}) W \mid x_p = x \rangle, \quad (39)$$

$$\mathbb{G}_I = - \sum_{p \in \mathcal{B}} \sum_{p \in \mathcal{B}_p} \int_{\mathcal{V}} \int_0^\infty \langle \mathbf{s}_p \odot \mathbf{P}_p \mathbf{c}_{pq} W \mid x_p = x + \alpha \mathbf{z}, x_q = x - (1 - \alpha) \mathbf{z} \rangle \otimes \mathbf{z} d\alpha d\mathbf{z}. \quad (40)$$

The internal orientation-couple density $\mathbf{N}$ and the internal mesofluctuations density $\mathbf{Z}$ are given by

$$\mathbf{N} = - \sum_{p \in \mathcal{B}} \langle I |\mathbf{s}_p|^2 \mathbf{d}_p \odot \mathbf{d}_p W \mid x_p = x \rangle, \quad (41)$$

$$\mathbf{Z} = - \sum_{p \in \mathcal{B}} 2 \langle I |\mathbf{s}_p|^2 \mathbf{d}_p \odot \mathbf{s}_p W \mid x_p = x \rangle. \quad (42)$$

The noninertial body-force per unit mass $\mathbf{b}$, noninertial body-couple per unit mass $\mathbf{B}$, noninertial orientation-couple per unit mass $\mathbf{M}$, and body-mesofluctuation per unit mass $\mathbf{J}$ are given by

$$\rho \mathbf{b} = \sum_{p \in \mathcal{B}} \langle \mathbf{f}_p^{\text{ni}} W \mid x_p = x \rangle, \quad (43)$$

$$\rho \mathbf{B} = \sum_{p \in \mathcal{B}} \langle \mathbf{d}_p \wedge c_p^{\text{ni}} W \mid x_p = x \rangle, \quad (44)$$

$$\rho \mathbf{M} = \sum_{p \in \mathcal{B}} \langle \mathbf{d}_p \odot \mathbf{P}_p \mathbf{c}_p^{\text{ni}} W \mid x_p = x \rangle, \quad (45)$$

$$\rho \mathbf{J} = \sum_{p \in \mathcal{B}} 2 \langle \mathbf{s}_p \odot \mathbf{P}_p \mathbf{c}_p^{\text{ni}} W \mid x_p = x \rangle. \quad (46)$$

The energy density e consists of the sum

$$e = e_K + e_I \quad (47)$$

of a kinetic contribution e_K and an interaction contribution e_I , with

$$e_K = \sum_{p \in \mathcal{B}} \left\langle \left(\frac{1}{2} m |\mathbf{v}_p|^2 + \frac{1}{2} I |s_p|^2 \right) W \mid x_p = x \right\rangle, \quad (48)$$

$$e_I = \frac{1}{2} \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}} \langle \psi_{pq} W \mid x_p = x \rangle. \quad (49)$$

The heat flux $\mathbf{q}$ is broken into a sum

$$\mathbf{q} = \mathbf{q}_{Kv} + \mathbf{q}_{Ks} + \mathbf{q}_T + \mathbf{q}_{If} + \mathbf{q}_{Ic} \quad (50)$$

of two kinetic contributions $\mathbf{q}_{Kv}$ and $\mathbf{q}_{Ks}$, a transport contribution $\mathbf{q}_T$, and two interaction contributions $\mathbf{q}_{If}$ and $\mathbf{q}_{Ic}$, with

$$\mathbf{q}_{Kv} = \sum_{p \in \mathcal{B}} \left\langle \frac{1}{2} m |\mathbf{v}_p - \mathbf{v}|^2 (\mathbf{v}_p - \mathbf{v}) W \mid x_p = x \right\rangle, \quad (51)$$

$$\mathbf{q}_{Ks} = \sum_{p \in \mathcal{B}} \left\langle \frac{1}{2} I |\mathbf{d}_p \odot \mathbf{S}_p - \dot{\mathbf{\Theta}} - \mathbf{\Delta}|^2 (\mathbf{v}_p - \mathbf{v}) W \mid x_p = x \right\rangle, \quad (52)$$

$$\mathbf{q}_T = \frac{1}{2} \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \langle \psi_{pq} (\mathbf{v}_p - \mathbf{v}) W \mid x_p = x \rangle, \quad (53)$$

$$\mathbf{q}_{If} = \frac{1}{2} \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_{\mathcal{V}} \int_0^\infty \langle [\mathbf{f}_{pq} \cdot \left(\frac{\mathbf{v}_p + \mathbf{v}_q}{2} - \mathbf{v} \right)] \mathbf{z} W \mid x_p = x + \alpha \mathbf{z}, x_q = x - (1 - \alpha) \mathbf{z} \rangle d\alpha d\mathbf{z}, \quad (54)$$

$$\mathbf{q}_{Ic} = \frac{1}{4} \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_{\mathcal{V}} \int_0^\infty \langle [(\mathbf{c}_{pq} \cdot \mathbf{s}_p - \mathbf{c}_{qp} \cdot \mathbf{s}_q) - (\mathbf{d}_p \odot \mathbf{P}_p \mathbf{c}_{pq} - \mathbf{d}_q \odot \mathbf{P}_q \mathbf{c}_{qp}) \cdot (\dot{\mathbf{\Theta}} + \mathbf{\Delta})] \mathbf{z} W \mid x_p = x + \alpha \mathbf{z}, x_q = x - (1 - \alpha) \mathbf{z} \rangle d\alpha d\mathbf{z}. \quad (55)$$

The radiation r is given by

$$r = \sum_{p \in \mathcal{P}} < \left(\mathbf{f}_p^{\text{ni}} \cdot (\mathbf{v}_p - \mathbf{v}) + \mathbf{d}_p \odot \mathbf{v}_p^{\text{ni}} \cdot (\mathbf{d}_p \odot \mathbf{s}_p - \dot{\Theta} - \Delta) \right) W |x_p = x>. \quad (56)$$

3.3 Decay properties

The above expressions involve improper integrals. To guarantee the convergence of these integrals, one must assume that W , the interaction energies, and the noninertial environmental terms decay rapidly at infinity. The following three conditions are sufficient to ensure that all of these integrals converge.

- There is a δ in $\mathbb{P}^\times$ such that for some y in $\mathcal{E}$ —and hence all y in $\mathcal{E}$ —the function Z defined by

$$Z(\sigma, t) := W(\sigma, t) \prod_{p \in \mathcal{B}} |x_p - y|^{4+\delta} \prod_{p \in \mathcal{B}} |\mathbf{v}_p|^{3+\delta} \prod_{p \in \mathcal{B}} |\mathbf{s}_p|^{2+\delta}, \text{ for all } \alpha \in \Sigma, t \in \mathcal{I},$$

(57)

and its partial derivatives are bounded by constants that depend only on time.

- The microscopic constitutive response function $\tilde{\psi}$ governing the interaction energy between rods and its partial derivatives are bounded.
- There are time-dependent scalars A and B such that

$$|\mathbf{f}_p^{\text{ni}}(t)| \leq A(t)|\mathbf{v}_p| + B(t), \quad |\nabla_{\mathbf{v}_p} \mathbf{f}_p^{\text{ni}}(t)| \leq A(t)|\mathbf{v}_p| + B(t), \quad (58)$$

$$|\mathbf{c}_p^{\text{ni}}(t)| \leq A(t)|\mathbf{s}_p| + B(t), \quad |\nabla_{\mathbf{s}_p} \mathbf{c}_p^{\text{ni}}(t)| \leq A(t)|\mathbf{s}_p| + B(t), \quad (59)$$

for all p in $\mathcal{B}$ and t in $\mathcal{Q}$.

Although these conditions resemble the three conditions of Noll [1], they differ in several ways. First, the third product on the right-hand side of (57) has no analog in the conditions of Noll [1] since his particles are unstructured. Also, the bounds (59) are absent from Noll's [1] conditions since his particles do not support couples. The one nontrivial alteration arises in the exponent of the first product on the right-hand side of (57). This exponent exceeds by unity the corresponding exponent of Noll [1]. This extra factor is needed because in the derivations below we take moments about a point y to obtain the moment of momentum balance while Noll [1] does not derive such a balance.

3.4 Discussion of the macroscopic balance laws

The macroscopic balance laws (11)–(17) deserve discussion and interpretation. In addition to comparisons with balances appearing in other macroscopic theories for liquid crystals, we provide a general discussion of our balances. The mass balance (11) and momentum balance (13) are standard in all conventional continuum theories, including those for liquid crystals, and, thus, require no comment.

3.4.1 Comparison with MacMillan's balances—Setting aside the mass and momentum balances, MacMillan's [23] theory for biaxial liquid crystals includes a moment of momentum balance

$$\rho\sigma(\Theta\ddot{\Theta} - \ddot{\Theta}\Theta) = \frac{1}{\sqrt{2}}(\mathbf{T}^\top - \mathbf{T}) + \text{div}(\Theta\mathbf{L} - \mathbf{L}\Theta) + \rho(\Theta\mathbf{M} - \mathbf{M}\Theta), \quad (60)$$

an orientation balance

$$\rho\sigma\ddot{\Theta} = \mathbf{N} + \text{div} \mathbf{L} + \rho\mathbf{M}, \quad (61)$$

and an energy balance

$$\dot{e} + e \text{div} \mathbf{v} + \text{div}(\mathbf{q} - \mathbf{T}^\top \mathbf{v} - \mathbf{L}^\top \dot{\Theta}) = \rho \mathbf{b} \cdot \mathbf{v} + \rho \mathbf{M} \cdot \dot{\Theta} + r. \quad (62)$$

Direct comparison shows that the balances (14)–(15) and (17) reduce to the balances of MacMillan's [23] theory for biaxial liquid crystals when

Δ , Π , $\mathbf{H}$, $\mathbf{Z}$, $\mathbf{G}$, and $\mathbf{J}$ are stipulated to vanish

(63)

and

$$\mathbf{S} = \Theta\dot{\Theta} - \dot{\Theta}\Theta, \quad \mathbf{C} = \Theta\mathbf{L} - \mathbf{L}\Theta, \quad \mathbf{B} = \Theta\mathbf{M} - \mathbf{M}\Theta. \quad (64)$$

The conditions (63)–(64) can be interpreted on the statistical level. The relative average rate arises because the time derivative of an average is not generally equal to the average of time derivatives, as can be seen from (26). Thus, this term being zero means that these two quantities agree. The orientation flux tensor Π measures the rate at which the tensor moment of inertia changes due to the redistribution of rods in space. Hence, neglecting Π corresponds to stipulating that rods do not migrate very rapidly. The terms $\mathbf{Z}$, $\mathbf{G}$, and $\mathbf{J}$ are all related to mesofluctuations. These terms can be neglected when the product of the spin and the resultant couple of each rod is sufficiently small. The Reynolds tensor $\mathbf{H}$ can be neglected when the square of the spin of each rod is sufficiently small. Finally, the relations

(64) hold if the averages of the underlying products are assumed to equal the products of the underlying averages.

3.4.2 Uniaxial specializations—MacMillan's [23] theory can describe liquid crystals that transition between biaxial, uniaxial, and isotropic states. Moreover, MacMillan [23] demonstrated that his orientation balance encompasses as a special case the director balance in the uniaxial theory of Ericksen [34] and Leslie [35]. An argument analogous to MacMillan's [23] can be applied to (15). Additionally, as Ericksen [36] states, his theory for uniaxial liquid crystals with variable orientation is a special case of MacMillan's [23] general theory. The balance laws (11)–(17) therefore also include this extended uniaxial theory as a special case. Specifically, to obtain Ericksen's [36] theory for uniaxial liquid crystals with variable degree of orientation, it suffices to constrain the orientation tensor to take the form

$$\Theta = \frac{S}{\sqrt{2}} \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \mathbf{1} \right) \quad (65)$$

where $\mathbf{n}$ is the director, a unit-vector order parameter, and S is the degree of orientation, a scalar order parameter; in (65), the factor $1/\sqrt{2}$ is present because of the way the circle product $\odot$ that appears in (23) is defined. Since $\mathbf{n}$ is constrained to be a unit vector, one must introduce reactions to guarantee that this constraint is satisfied. The variable S is called the degree of orientation and since $3\sqrt{2}\Theta + \mathbf{1}$ is positive definite, S must satisfy

$$-\frac{1}{2} < S < 1. \quad (66)$$

The value $S = 0$ corresponds to an isotropic state. Thus, Ericksen's [36] theory can describe liquid crystals that transition between uniaxial and isotropic states. On assuming that S is constant, Ericksen's [36] theory specializes to the conventional director theory of Ericksen [28] and Leslie [35]. Ericksen's [36] extended theory also allows for the description of point and line defects.

3.4.3 General discussion—Some general comments on the balances (12) and (14)–(16) are also in order. Setting aside the tensor moment of inertia (12) until later, consider the moment of momentum balance (14). In traditional continuum theories, this balance implies the stress tensor $\mathbf{T}$ is symmetric. Because of the non-standard terms that appear in (14), $\mathbf{T}$ need not be symmetric here. The non-standard terms appearing in (14) can be interpreted as follows: the one on the left-hand side is an inertial term due to the rotation of the tensor order parameter, the third term on the right-hand side is due to surface couples, and the last term on the right-hand side is due to external couples.

The orientation balance (15) governs the evolution of the orientation tensor Θ which, as was discussed above, generalizes the director balance present in earlier theories of liquid crystals. As was noted previously, (15) differs from the corresponding balance found by MacMillan

[23] because of the presence of the relative average rate (via its time rate $\dot{\cdot}$) and the Reynolds tensor $\mathbf{H}$. Both of these quantities are inertial in nature and are governed by their own balance laws. Whereas the relative average rate is governed by the tensor moment of inertia balance (12), the Reynolds tensor $\mathbf{H}$ is governed by the mesofluctuation balance (16). Neither of these balances are standard in continuum theories for liquid crystals as formulated by Lubensky [26], Müller [29], or MacMillian [23]. However, they do have precedents elsewhere. The tensor moment of inertia balance agrees with that of Pitteri [4] and a mesofluctuation balance appears in Capriz's [30] theory of ephemeral continua.

Bearing in mind (23), notice that the orientation tensor Θ is a traceless and symmetric measure of the extent to which the state of the liquid crystal differs from isotropic (see, for example, Ericksen [36] or Virga [37]). By (26), (35)–(37), and (45), ρ , $\text{div } \mathbf{L}$, and $\mathbf{M}$ are traceless. Moreover, by (27) and (41), the trace of $\rho \sigma \mathbf{H}$ is equal to that of $\mathbf{N}$ and, thus, the orientation balance (15) governs only the traceless part of Θ .

The field equations (11)–(17) are not sufficient to determine the fields ρ , $\mathbf{v}$, Θ , and $\mathbf{H}$, which are the unknowns to be determined. To rectify this, it would be necessary to introduce constitutive laws. Here our goal is to derive the balances (11)–(17), not to solve initial-boundary-value problems based on them. We make no attempt to formulate such constitutive laws here.

4 Derivation of expected values

Consider a rod p in $\mathcal{B}$. Let $\mathbf{g}_p : \Omega \rightarrow \mathcal{W}$, with $\mathcal{W}$ a finite-dimensional linear space, be a state function that describes some physical quantity associated with p . For example, $\mathbf{g}_p$ might be the momentum $m\mathbf{v}_p$ of the rod p . The value

$$\langle \mathbf{g}_p W | x_p = x \rangle \quad (67)$$

represents the probability density of the physical quantity for the rod p when the rod is at position x in $\mathcal{E}$. Hence, the total probability density of the quantity $\mathbf{g}_p$ for the system $\mathcal{B}$ at x is

$$\sum_{p \in \mathcal{B}} \langle \mathbf{g}_p W | x_p = x \rangle. \quad (68)$$

Similarly, the probability density of the quantity $\mathbf{g}_p$ for the rod p when p is at x and rod q is at $\tilde{x}$ in $\mathcal{E}$ is given by

$$\langle \mathbf{g}_p W | x_p = x, x_q = \tilde{x} \rangle. \quad (69)$$

For what remains of this section, let $\mathcal{A}$ be a regular region in $\mathcal{E}$. We denote by $\partial \mathcal{A}$ the boundary of $\mathcal{A}$ and let $\mathbf{n} : \partial \mathcal{A} \rightarrow \text{Usph}(\mathcal{V})$ be the mapping that gives the exterior unit normal on $\partial \mathcal{A}$.

4.1 Density, momentum, orientation tensor, and orientation flux tensor

It follows from (68) that (21) and (22) represent the expected values for the mass density ρ and velocity $\mathbf{v}$, respectively.

Given a rod p in $\mathcal{B}$, $\mathbf{d}_p \odot \mathbf{d}_p$ describes the orientation of p , neglecting the distinction between $\mathbf{d}_p$ and $-\mathbf{d}_p$. Thus, by (68), (23) gives the probability density of the expected value of the orientation of the system. The factor of one half appearing in (23) makes the macroscopic balances match the more traditional balance for liquid crystals, such as those found by MacMillan [23].

Since $\mathbf{d}_p \odot \mathbf{d}_p$ describes the orientation of the rod p , it follows from (24) that

$$\int_{\partial \mathcal{A}} \Pi \mathbf{n} dA$$

(70)

gives the rate of change of the total orientation in $\mathcal{A}$ due to rods entering and exiting the boundary of $\mathcal{A}$. Here one must keep in mind that the velocity $\mathbf{v}$ and orientation Θ , as given by (21)–(23), are defined pointwise in $\mathcal{A}$.

4.2 Spin, relative average rate, and Reynolds tensor

Since

$$\langle I \mathbf{d}_p \wedge \mathbf{s}_p W | x_p = x \rangle \quad (71)$$

gives the expected value of the density of spin, or rate of rotation, of the rod p when it is at x , it follows that (25) gives the expected value of the density of spin $\mathbf{S}$.

Moreover, since $\mathbf{d}_p \odot \mathbf{s}_p$ gives the rate of change of the orientation of rod p , it follows from (68) that

$$\sum_{p \in \mathcal{B}} \langle m \mathbf{d}_p \odot \mathbf{s}_p W | x_p = x \rangle \quad (72)$$

gives the expected value of the rate of change of the orientation tensor weighted with the mass density. Thus, by (26), reckons the difference between the rate of change of the expected value of the orientation and the expected value of the rate of change of the orientation.

In theories for turbulent fluid flow, the Reynolds tensor is defined as the average of the circle product of the fluctuating part of the velocity with itself. Building upon this notion, Capriz [30] obtained a Reynolds tensor by averaging the tensor product of a mesoscopic velocity

with itself. In the present context, the mesoscopic velocity can be identified with the spin $\mathbf{s}_p$ of the rods. Thus, (27) gives the expected value of the Reynolds tensor.

4.3 Stress tensor

The stress tensor is characterized by the property that the total force $\mathbf{f}(\mathcal{A})$ exerted on $\mathcal{A}$ by $\mathcal{E}$ across $\mathcal{A}$ is given by

$$\mathbf{f}(\mathcal{A}) = \int_{\partial\mathcal{A}} \mathbf{T} \mathbf{n} dA. \quad (73)$$

This total force on $\mathcal{A}$ is the sum of two contributions: the kinetic force $\mathbf{f}_K(\mathcal{A})$ coming from the rate of change of momentum of $\mathcal{A}$ due to rods entering and exiting $\mathcal{A}$ and the interaction force $\mathbf{f}_I(\mathcal{A})$ coming from rods outside of $\mathcal{A}$ exerting forces on rods inside of $\mathcal{A}$.

One can see that

$$\mathbf{f}_K(\mathcal{A}) = \int_{\partial\mathcal{A}} \mathbf{T}_K \mathbf{n} dA \quad (74)$$

gives the kinetic force that corresponds to the rate of change of the momentum of $\mathcal{A}$ as rods enter and exit $\mathcal{A}$ through $\mathcal{A}$. Here, one must keep in mind that the velocity $\mathbf{v}$ is defined pointwise in $\mathcal{A}$.

Given rods p and q in $\mathcal{E}$, by (69),

$$\int_{\mathcal{A}} \int_{\mathcal{E}} \langle \mathbf{f}_{pq} W | x_p = x, x_q = \tilde{x} \rangle d\tilde{x} dx \quad (75)$$

gives the expected value of the force of rod q in $\mathcal{E}$ on rod p in $\mathcal{A}$. Summing over all p and q , we obtain the total interaction force

$$\mathbf{f}_I(\mathcal{A}) = \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_q} \int_{\mathcal{A}} \int_{\mathcal{E}} \langle \mathbf{f}_{pq} W | x_p = x, x_q = \tilde{x} \rangle d\tilde{x} dx \quad (76)$$

exerted by all rods on rods in $\mathcal{A}$. We may use a lemma due to Pitteri [38] and (30) to find that

$$\mathbf{f}_I(\mathcal{A}) = -\frac{1}{2} \int_{\partial\mathcal{A}} \left(\sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_q} \int_{\gamma} \int_0^\infty \langle \mathbf{f}_{pq} W | x_p = x + \alpha \mathbf{z}, x_q = x - (1 - \alpha) \mathbf{z} \rangle \otimes \mathbf{z} d\alpha d \right) \mathbf{n} dA = \int_{\partial\mathcal{A}} \mathbf{T}_I \mathbf{n} dA. \quad (77)$$

In view of (28), (74), and (77), we obtain (73).

4.4 Couple tensor

The couple tensor $\mathbb{C}$ is characterized by the property that the total torque on $\mathcal{A}$ from $\mathcal{E}$ through $\mathcal{A}$ not due to forces is given by

$$\int_{\partial\mathcal{A}} \mathbb{C} \mathbf{n} dA. \quad (78)$$

The couple tensor is the sum of three terms: a kinetic contribution due to the rate of change of the spin of $\mathcal{A}$ due to rods entering or exiting $\mathcal{A}$, an interaction contribution due to resultant forces on rods in $\mathcal{A}$ from those outside of $\mathcal{A}$, and an interaction contribution due to resultant couples on rods in $\mathcal{A}$ from those outside of $\mathcal{A}$.

One can see that

$$\int_{\partial\mathcal{A}} \mathbb{C}_K \mathbf{n} dA \quad (79)$$

gives the kinetic torque acting on $\mathcal{A}$ from $\mathcal{E} \setminus \mathcal{A}$ due to the rate of change of spin in $\mathcal{A}$ due to rods entering and exiting $\mathcal{A}$ through $\mathcal{A}$. Here, one must keep in mind that the velocity $\mathbf{v}$ and spin $\mathbf{S}$ are defined pointwise in $\mathcal{A}$.

Using an argument similar to that leading to (77), we find that the total interaction torque $\mathbf{R}_I(\mathcal{A}; y)$ on $\mathcal{A}$ from $\mathcal{E}$ about y in $\mathcal{E}$ due to torques on rods in $\mathcal{A}$ from those outside of $\mathcal{A}$ about y is given by

$$\mathbf{R}_I(\mathcal{A}; y) = -\frac{1}{2} \int_{\partial\mathcal{A}} \left(\sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_{\mathcal{V}} \int_0^\infty \langle \mathbf{R}_{pq}(y) W | x_p = x + \alpha \mathbf{z}, x_q = x - (1 - \alpha) \mathbf{z} \rangle \otimes \mathbf{z} d\alpha \right) \mathbf{n} dA. \quad (80)$$

When $x_p = x + \alpha \mathbf{z}$, we have, by the definition of $\mathbf{R}_{pq}(y)$,

$$\mathbf{R}_{pq}(y) = (x - y) \wedge \mathbf{f}_{pq} + \alpha \mathbf{z} \wedge \mathbf{f}_{pq} + \mathbf{d}_p \wedge \mathbf{c}_{pq}. \quad (81)$$

Putting (81) into (80) and using (30), (33), and (34), we find that

$$\mathbf{R}_I(\mathcal{A}, y) = \int_{\partial\mathcal{A}} (x - y) \wedge (\mathbf{T}_I \mathbf{n}) dA + \int_{\partial\mathcal{A}} (\mathbb{C}_{IF} + \mathbb{C}_{IC}) \mathbf{n} dA. \quad (82)$$

The first term on the right-hand side of (82) is the total interaction torque on $\mathcal{A}$ from $\mathcal{E}$ about y due to the forces on $\mathcal{A}$ from $\mathcal{E}$. Thus, $\mathbb{C}_{IF} + \mathbb{C}_{IC}$ is the interaction couple stress. The terms $\mathbb{C}_{IF}$ and $\mathbb{C}_{IC}$ represent the contributions due to the resultant forces between rods and the resultant couples between rods, respectively.

In view of (31), (79), and (82), we have (78).

4.5 Internal orientation-couples and orientation-couple tensor

We now seek to justify the formulas for the internal orientation-couple density $\mathbf{N}$ and the orientation-couple tensor $\mathbb{L}$. These are characterized by the property that the total orientation-couple $\mathbf{C}(\mathcal{A})$ on $\mathcal{A}$ from $\mathcal{E}$ is given by

$$\mathbf{C}(\mathcal{A}) = \int_{\mathcal{A}} \mathbf{N} d\mathcal{V} + \int_{\partial\mathcal{A}} \mathbb{L} \mathbf{n} dA \quad (83)$$

The orientation-couple tensor is the sum of two terms: a kinetic contribution due to the rate of change of the orientation of $\mathcal{A}$ due to rods entering and exiting $\mathcal{A}$ and an interaction contribution due to orientation couples on rods in $\mathcal{A}$ from those outside of $\mathcal{A}$.

A noteworthy consequence of the balance of torques obtained by Seguin & Fried [32] is

$$\sum_{p \in \mathcal{P}} \frac{1}{2} I \overline{\dot{\mathbf{d}}_p \odot \dot{\mathbf{d}}_p} - \sum_{p \in \mathcal{P}} I \mathbf{s}_p \odot \mathbf{s}_p = - \sum_{p \in \mathcal{P}} I |\mathbf{s}_p|^2 \mathbf{d}_p \odot \mathbf{d}_p + \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{B}_p} \mathbf{d}_p \odot \mathbf{P}_p \mathbf{c}_{pq} + \sum_{p \in \mathcal{P}} \mathbf{d}_p \odot \mathbf{P}_p \mathbf{c}_p^{\text{ni}}, \quad (84)$$

which can be viewed a microscopic precursor of the orientation balance. In support of this assertion, consider the terms on the right-hand side of (84), which can be interpreted as follows: the first term gives inertial couples due to the magnitude of the spin of the rods in the system, the second term gives the orientation couples coming from rods in the system $\mathcal{B}$ due to resultant couples between rods, and the third term gives the orientation couples coming from noninertial environmental influences. The balance (84) is analogous to the microscopic balances Svendsen [5] obtained for higher-order velocity moments.

Motivated by (84) and bearing in mind (69) and (41), we see that

$$\int_{\mathcal{A}} \mathbf{N} d\mathcal{V} \quad (85)$$

gives the internal orientation-couples acting on $\mathcal{A}$.

One can see that

$$\mathbf{C}_K(\mathcal{A}) = \int_{\partial\mathcal{A}} \mathbb{L}_K \mathbf{n} dA \quad (86)$$

gives the kinetic orientation-couple that corresponds to the rate of change of the orientation of $\mathcal{A}$ as rods enter and exit $\mathcal{A}$ through $\mathcal{A}$. Here, one must keep in mind that the velocity $\mathbf{v}$ and orientation rate of change $\dot{\mathbf{\Theta}}$ are defined pointwise in $\mathcal{A}$.

Motivated by (84) and bearing in mind (69), we see that

$$\mathbf{C}_1(\mathcal{A}) = \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_{\mathcal{A}} \int_{\mathcal{E}} \langle \mathbf{d}_p \odot \mathbf{P}_p \mathbf{c}_{pq} W | x_p = x, x_q = \tilde{x} \rangle d\tilde{x} dx \quad (87)$$

is the expected value of the total orientation-couple on $\mathcal{A}$ due to both the internal orientation-couple density and the interaction part of the orientation-couple tensor. We may use a lemma due to Pitteri [38] and (37) to obtain

$$\mathbf{C}_1(\mathcal{A}) = \int_{\partial \mathcal{A}} \left(-\frac{1}{2} \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_{\mathcal{V}} \int_0^\infty \langle \mathbf{d}_p \odot \mathbf{P}_p \mathbf{c}_{pq} W | x_p = x + \alpha \mathbf{z}, x_q = x - (1 - \alpha) \mathbf{z} \rangle \otimes \mathbf{z} d\alpha d\mathbf{z} \right) \mathbf{n} dA = \int_{\partial \mathcal{A}} \mathbb{L}_1 \mathbf{n} dA, \quad (88)$$

from which it follows that $\mathbb{L}_1$ generate the total interaction contribution due to orientation couples on $\mathcal{A}$.

In view of (35), (85), (86), and (88), we obtain (83).

4.6 Internal mesofluctuations and power-flux tensor

We now seek to justify the formulas for the internal orientation-couple density $\mathbf{Z}$ and the power-flux tensor $\mathbb{G}$. These are characterized by the property that the total mesofluctuation $\mathbf{F}(\mathcal{A})$ on $\mathcal{A}$ from $\mathcal{E}$ is given by

$$\mathbf{F}(\mathcal{A}) = \int_{\mathcal{A}} \mathbf{Z} d\mathcal{V} + \int_{\partial \mathcal{A}} \mathbb{G} \mathbf{n} dA \quad (89)$$

The power-flux tensor is the sum of two terms: a kinetic contribution due to the rate of change of the Reynolds tensor within $\mathcal{A}$ due to rods entering and exiting $\mathcal{A}$ and an interaction contribution due to tensor power expenditures on rods in $\mathcal{A}$ from those outside of $\mathcal{A}$.

Another noteworthy consequence of the balance of torques obtained by Seguin & Fried [32], similar to that of (84), is

$$\sum_{p \in \mathcal{P}} I \overline{\mathbf{s}_p \odot \dot{\mathbf{s}}_p} = - \sum_{p \in \mathcal{P}} 2I |\mathbf{s}_p|^2 \mathbf{d}_p \odot \mathbf{s}_p + \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{B}_p} 2\mathbf{s}_p \odot \mathbf{P}_p \mathbf{c}_{pq} + \sum_{p \in \mathcal{P}} 2\mathbf{s}_p \odot \mathbf{P}_p \mathbf{c}_p^{\text{ni}}. \quad (90)$$

Whereas (84) is a microscopic precursor of the orientation balance, (90) is a microscopic precursor of what, following Capriz [30] and Brocato & Capriz [31], we call the mesofluctuation balance. The terms in (90) can be given analogous interpretations to those

in (84) and are called mesofluctuations. As with (84), (90) is analogous to the microscopic balances Svendsen [5] obtained for higher-order velocity moments.

Motivated by (90) and bearing in mind (69) and (42), we see that

$$\int_{\mathcal{A}} \mathbf{Z} d\mathcal{V} \quad (91)$$

gives the internal mesofluctuations acting on $\mathcal{A}$.

One can see that

$$\mathbf{F}_K(\mathcal{A}) = \int_{\partial\mathcal{A}} \mathbb{G}_K \mathbf{n} dA \quad (92)$$

gives the mesofluctuation that corresponds to the in flux of the tensor power of $\mathcal{A}$ as rods enter and exit $\mathcal{A}$ through $\mathcal{A}$. Here one must keep in mind that the velocity $\mathbf{v}$ and Reynolds tensor $\mathbf{H}$ are defined pointwise in $\mathcal{A}$.

Motivated by (90) and bearing in mind (69), we see that

$$\mathbf{F}_I(\mathcal{A}) = \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_{\mathcal{A}} \int_{\mathcal{E}} \langle 2\mathbf{s}_p \odot \mathbf{P}_p \mathbf{c}_{pq} W | x_p = x, x_q = \tilde{x} \rangle d\tilde{x} dx \quad (93)$$

is the expected value of the interaction contribution due to the power-flux tensor. Using an argument analogous to leading to (88) but invoking (40) instead (37), we find that

$$\mathbf{F}_I(\mathcal{A}) = \int_{\partial\mathcal{A}} \mathbb{G}_I \mathbf{n} dA, \quad (94)$$

from which it follows that $\mathbb{G}_I$ generate the interaction contribution due to mesofluctuations on $\mathcal{A}$.

In view of (38), (91), (92), and (94), we obtain (89).

4.7 Noninertial body-forces, couples, orientation-couples, and mesofluctuations

As a consequence of (68), (43) gives the expected value for the noninertial body-force density.

Let $\mathbf{R}^{\text{ni}}(\mathcal{A}; y)(x)$ denote the expected value for the noninertial body-torque density about y in $\mathcal{E}$ at x in $\mathcal{E}$. By (68), we have

$$\mathbf{R}^{\text{ni}}(\mathcal{A}; y)(x) = \sum_{p \in \mathcal{B}} \langle \mathbf{R}_p^{\text{ni}}(y) W | x_p = x \rangle. \quad (95)$$

Using the definition of $\mathbf{R}_p^{\text{ni}}(y)$, (43), and (44) we have

$$\mathbf{R}^{\text{ni}}(\mathcal{A}; y)(x) = (x - y) \wedge \rho(x) \mathbf{b}(x) + \rho(x) \mathbf{B}(x), \quad (96)$$

from which it follows that $\mathbf{B}$ represents the expected value for the noninertial body-torque density that does not come from forces—that is, the noninertial body-couple density.

From (84), we know that $\mathbf{d}_p \odot \mathbf{P}_p \mathbf{c}_p^{\text{ni}}$ is related to the noninertial orientation-couple acting on rod p . We see, by (68), that (45) gives the probability density of the noninertial orientation-couple density. Similarly, motivated by (90), we see that (46) gives the probability density of the noninertial mesofluctuation density.

4.8 Energy density

Since $k_p = \frac{1}{2}m|\mathbf{v}_p|^2 + \frac{1}{2}I|\mathbf{s}_p|^2$ is the kinetic energy of a rod p , it follows from (68) that (48) is the probability density of the kinetic-energy density.

Let p and q be rods at x_p and x_q respectively. We assume that the interaction energy ψ_{pq} is distributed evenly between the points x_p and x_q so that the total interaction-energy at x_p is

$$\psi_p := \frac{1}{2} \sum_{q \in \mathcal{B}_p} \psi_{pq}. \quad (97)$$

Thus, by (68), (49) gives the probability density of the interaction-energy density.

The energy density is the sum of the kinetic energy and the interaction energy so (47) gives the probability density of the energy density.

4.9 Heat flux

The heat flux $\mathbf{q}$ is characterized by the property that the total energy $q(\mathcal{A})$ transferred to $\mathcal{A}$ from $\mathcal{E}$ through $\mathcal{A}$ is given by

$$q(\mathcal{A}) = \int_{\partial \mathcal{A}} \mathbf{q} \cdot \mathbf{n} dA. \quad (98)$$

We show that $\mathbf{q}$ is the sum of five terms, two of which result from the influx of kinetic energy, one of which results from the influx of interaction energy, and the last two of which result from power expenditures.

Using (68), one can see that

$$\int_{\partial \mathcal{A}} \mathbf{q}_{\text{Kv}} \cdot \mathbf{n} dA \quad (99)$$

gives the energy transferred to $\mathcal{A}$ due to the kinetic energy associated with the velocity of rods entering $\mathcal{A}$ through $\mathcal{A}$. Here, one must keep in mind that the velocity $\mathbf{v}$ is defined pointwise in $\mathcal{A}$.

Recall that the kinetic energy of a rod p associated with the rate of change of its director is

$\frac{1}{2}I|\mathbf{s}_p|^2$, which, since $\mathbf{d}_p \cdot \mathbf{s}_p = 0$, can be rewritten as

$$\frac{1}{2}I|\mathbf{s}_p|^2 = \frac{1}{2}I|\mathbf{d}_p \odot \mathbf{s}_p|^2. \quad (100)$$

Thus, using (68), one finds that

$$\int_{\partial\mathcal{A}} \mathbf{q}_{\text{Ks}} \cdot \mathbf{n} dA \quad (101)$$

gives the energy transferred to $\mathcal{A}$ due to the kinetic energy associated with the rotation of rods entering $\mathcal{A}$ through $\mathcal{A}$. Here, one must keep in mind that the velocity $\mathbf{v}$ and orientation rate of change $\dot{\mathbf{\Theta}}$ are defined pointwise in $\mathcal{A}$.

Notice that, on using (97), (53) can be written as

$$\mathbf{q}_T = \sum_{p \in \mathcal{B}} \langle \psi_p(\mathbf{v}_p - \mathbf{v})W \mid x_p = x \rangle. \quad (102)$$

From (102) and the discussions in the previous two paragraphs, it should be clear that

$$\int_{\partial\mathcal{A}} \mathbf{q}_T \cdot \mathbf{n} dA \quad (103)$$

represents the energy transferred to $\mathcal{A}$ from rods entering $\mathcal{A}$. Here, one must keep in mind that the velocity $\mathbf{v}$ is defined pointwise in $\mathcal{A}$.

Consider

$$\mathbf{q}_{\text{If}}^* := \mathbf{q}_{\text{If}} - \mathbf{T}_I^\top \mathbf{v} = \frac{1}{2} \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_{\mathcal{V}} \int_0^\infty \langle [\mathbf{f}_{pq}(\mathbf{v}_p + \mathbf{v}_q)] \mathbf{z} W \mid x_p = x + \alpha \mathbf{z}, x_q = x - (1 - \alpha) \mathbf{z} \rangle d\alpha d\mathbf{z}.$$

(104)

and

$$\mathbf{q}_{\text{Ic}}^* := \mathbf{q}_{\text{Ic}} - \mathbb{L}_{\text{I}}^\top \dot{\boldsymbol{\Theta}} + \boldsymbol{\Delta} = \frac{1}{4} \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_{\mathcal{V}} \int_0^\infty \langle [\mathbf{c}_{pq} \cdot \mathbf{s}_p - \mathbf{c}_{pq} \cdot \mathbf{s}_q] \mathbf{z} W \mid x_p = x + \alpha \mathbf{z}, x_q = x - (1 - \alpha) \mathbf{z} \rangle d\alpha d\mathbf{z}. \quad (105)$$

We start by showing that

$$\int_{\partial \mathcal{A}} (\mathbf{q}_{\text{If}}^* + \mathbf{q}_{\text{Ic}}^*) \cdot \mathbf{n} dA \quad (106)$$

represents the energy transferred to $\mathcal{A}$ due to power expended by the rods outside of $\mathcal{A}$ on the rods in $\mathcal{A}$ in the absence of external influences. As with the interaction energy, we assume that the power expended on a rod p by a rod q is divided equally between the two locations of the rods. Thus, given a state of the system $\mathcal{B}$, and letting $\mathcal{P}$ denote the subsystem of rods inside $\mathcal{A}$, the total power expended inside of $\mathcal{A}$, excluding that due to environmental influences, is given by

$$P_{\text{int}}(\mathcal{P}) + \frac{1}{2} \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} (\mathbf{f}_{pq} \cdot \mathbf{v}_p + \mathbf{c}_{pq} \cdot \mathbf{s}_p) + \frac{1}{2} \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} (\mathbf{f}_{qp} \cdot \mathbf{v}_q + \mathbf{c}_{qp} \cdot \mathbf{s}_q). \quad (107)$$

In (107), the first term is the power expended due to interactions between rods inside of $\mathcal{A}$, the second term is the power expended associated with the resultant forces and couples from rods outside of $\mathcal{A}$ acting on rods inside of $\mathcal{A}$, and the third term is the power expended associated with the resultant forces and couples from rods inside of $\mathcal{A}$ acting on rods outside of $\mathcal{A}$. On using the balance of power for $\mathcal{P}$ (see (100) of Seguin & Fried [32]), in the absence of environmental influences, (107) can be expressed as

$$-\frac{1}{2} \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} (\mathbf{f}_{pq} \cdot \mathbf{v}_p - \mathbf{f}_{qp} \cdot \mathbf{v}_q + \mathbf{c}_{pq} \cdot \mathbf{s}_p - \mathbf{c}_{qp} \cdot \mathbf{s}_q). \quad (108)$$

Hence, by (69),

$$-\int_{\mathcal{A}} \int_{\mathcal{E} \setminus \mathcal{A}} \sum_{p \in \mathcal{P}} \sum_{q \in \mathcal{P}'} \langle \frac{1}{2} (\mathbf{f}_{pq} \cdot \mathbf{v}_p - \mathbf{f}_{qp} \cdot \mathbf{v}_q + \mathbf{c}_{pq} \cdot \mathbf{s}_p - \mathbf{c}_{qp} \cdot \mathbf{s}_q) W \mid x_p = x, x_q = \tilde{x} \rangle d\tilde{x} dx \quad (109)$$

represents the energy transferred to $\mathcal{A}$ due to the power expended by rods outside of $\mathcal{A}$ on rods inside of $\mathcal{A}$. Using a lemma due to Pitteri [38], (104), and (105), we find that (109) is equal to (106).

The energy transferred encompassed by (106) includes the energy that is transferred to $\mathcal{A}$ due to macroscopic forces and couples—that is, due to the stress $\mathbf{T}_I$ and the orientation couple stress $\mathbb{L}_I$. To obtain the interaction energy transferred due purely to microscopic effects, we must subtract off the macroscopic effects. Since the macroscopic energy transferred to $\mathcal{A}$ through $\mathcal{A}$ is given by

$$-\int_{\partial\mathcal{A}}(\mathbf{T}_I \mathbf{n} \cdot \mathbf{v} + \mathbb{L}_I \mathbf{n} \cdot (\dot{\mathbf{\Theta}} + \mathbf{\Delta}))dA, \quad (110)$$

the purely microscopic energy transferred to $\mathcal{A}$ through $\mathcal{A}$, using (104) and (105), is given by

$$\int_{\partial\mathcal{A}}(\mathbf{q}_{If}^* + \mathbf{q}_{Ic}^*) \cdot \mathbf{n} dA - \left(-\int_{\partial\mathcal{A}}(\mathbf{T}_I \mathbf{n} \cdot \mathbf{v} + \mathbb{L}_I \mathbf{n} \cdot (\dot{\mathbf{\Theta}} + \mathbf{\Delta}))dA\right) = \int_{\partial\mathcal{A}}(\mathbf{q}_{If} + \mathbf{q}_{Ic}) \cdot \mathbf{n} dA. \quad (111)$$

In view of (50), (99), (101), (103), and (111), we obtain (98).

4.10 Radiation

It follows from (68) that

$$r^* := \sum_{p \in \mathcal{B}} \langle (\mathbf{f}_p^{\text{ni}} \cdot \mathbf{v}_p + \mathbf{c}_p^{\text{ni}} \cdot \mathbf{s}_p) W \mid x+p=x \rangle \quad (112)$$

is the expected value of the density of the rate of change of the energy due to environmental influences. This includes the radiation as well as the power expenditures associated with the noninertial body-force density $\mathbf{b}$ and the noninertial orientation-couple density $\mathbf{M}$. Thus, by subtracting these power expenditures from r^* and using (56) and the identity $\mathbf{d}_p \cdot \mathbf{s}_p = 0$, we obtain the relation

$$r = r^* = \rho \mathbf{b} \cdot \mathbf{v} - \rho \mathbf{M} \cdot (\dot{\mathbf{\Theta}} + \mathbf{\Delta}) \quad (113)$$

for the radiation.

5 Derivations of the balance laws

Each of the balance laws (11)–(17) is derived using the same general procedure. Having identified a microscopic quantity for a rod p associated with the macroscopic balance law to be derived,¹ the steps involved are essentially as follows:

1. Multiply the Liouville equation (8) by the microscopic quantity under consideration, integrate over Ω_p , and set x_p equal to x .

¹For example, to derive the momentum balance, the relevant microscopic quantity for a rod p is the momentum $m\mathbf{v}_p$ of the rod.

2. Integrate by parts, possibly many times, use identities involving the divergence to simplify the resulting equation, and sum the simplified equation over all rods p in $\mathcal{B}$.
3. Identify the terms in the resulting macroscopic equation as expected values of the state functions.

5.1 Mass balance

Let p in $\mathcal{B}$ be given. Multiply (8) by m , integrate over Ω_p , and set $x_p = x$ to obtain

$$0 = \langle mW' \mid x_p = x \rangle + \sum_{q \in \mathcal{B}} \left[\langle m(\nabla_{x_q} W \cdot \mathbf{v}_q) \mid x_p = x \rangle + \langle \operatorname{div}_{\mathbf{v}_q} (W(-\nabla_{x_q} \psi + \mathbf{f}_q^{\text{ni}})) \mid x_p = x \rangle + \langle m(\nabla_{\mathbf{d}_q} W \cdot \mathbf{s}_q) \mid x_p = x \rangle + \langle \frac{m}{I} \operatorname{div}_{\mathbf{s}_q} (W \mathbf{P}_q) \mid x_p = x \rangle \right] \quad (114)$$

Bearing in mind that $m\mathbf{v}_q$ is independent of x_q , integrate by parts with respect to x_q for $q \neq p$, to give

$$\langle m(\nabla_{x_q} W \cdot \mathbf{v}_q) \mid x_p = x \rangle = 0. \quad (115)$$

For similar reasons, integrate by parts with respect to $\mathbf{v}_q$, $\mathbf{d}_q$, and $\mathbf{s}_q$ to give

$$\langle \nabla_{\mathbf{v}_q} W \cdot \nabla_{x_q} \psi \mid x_p = 0 \rangle = 0, \quad (116)$$

$$\langle m(\nabla_{\mathbf{d}_q} W \cdot \mathbf{s}_q) \mid x_p = x \rangle = 0, \quad (117)$$

and

$$\langle \frac{m}{I} (\nabla_{\mathbf{s}_q} W \cdot \mathbf{P}_q \nabla_{\mathbf{d}_q} \psi) \mid x_p = x \rangle = 0, \quad (118)$$

respectively, for all q . Furthermore, integrate by parts with respect to $\mathbf{v}_q$ to give

$$\langle \operatorname{div}_{\mathbf{v}_q} (W \mathbf{f}_q^{\text{ni}}) \mid x_p = x \rangle = 0 \quad (119)$$

and integrate by parts with respect to $\mathbf{s}_q$ to give

$$\langle \frac{m}{I} \text{div}_{\mathbf{s}_q} (W \mathbf{P}_q \mathbf{c}_q^{\text{ni}}) \mid x_p = x \rangle = 0. \quad (120)$$

In view of (115)–(120), (114) becomes

$$0 = \langle m W' \mid x_p = x \rangle + \langle m (\nabla_{x_p} W \cdot \mathbf{v}_p) \mid x_p = x \rangle. \quad (121)$$

Since m and $\mathbf{v}_p$ do not depend on x_p , an identity involving the divergence implies that $\text{div}_{x_p} (m \mathbf{v}_p W) = m \nabla_{x_p} W \cdot \mathbf{v}_p$. With this identity, summing (121) over all p in $\mathcal{B}$ gives

$$0 = \left(\sum_{p \in \mathcal{B}} \langle m W \mid x_p = x \rangle \right)' + \text{div}_x \left(\sum_{p \in \mathcal{B}} \langle m \mathbf{v}_p W \mid x_p = x \rangle \right). \quad (122)$$

Finally, to obtain the mass balance (11), use the identifications (21) and (22) in (122), as well as the identity $\dot{\rho} = \rho' + \nabla \rho \cdot \mathbf{v}$.

5.2 Tensor moment of inertia balance

Let p in $\mathcal{B}$ be given. Multiply (8) by $\mathbf{Y}_p = \sigma m (\mathbf{1} - \mathbf{d}_p \otimes \mathbf{d}_p)$, integrate over Ω_p , and set $x_p = x$ to obtain

$$0 = \langle \mathbf{Y}_p W' \mid x_p = x \rangle + \sum_{q \in \mathcal{B}} \left[\langle \mathbf{Y}_p (\nabla_{x_q} W \cdot \mathbf{v}_q) \mid x_p = x \rangle + \langle \frac{\mathbf{Y}_p}{m} \text{div}_{\mathbf{v}_q} (W (-\nabla_{x_q} \psi + \mathbf{f}_q^{\text{ni}})) \mid x_p = x \rangle + \langle \mathbf{Y}_p (\nabla_{\mathbf{d}_p} W \cdot \mathbf{s}_q) \mid x_p = x \rangle + \langle \frac{\mathbf{Y}}{I} \right. \\ \left. \right] \quad (123)$$

Integrate by parts, dropping terms that vanish, to leave

$$0 = \langle \mathbf{Y}_p W' \mid x_p = x \rangle + \langle \mathbf{Y}_p (\nabla_{x_p} W \cdot \mathbf{v}_p) \mid x_p = x \rangle + \langle I (\mathbf{d}_p \otimes \mathbf{s}_p + \mathbf{s}_p \otimes \mathbf{d}_p) W \mid x_p = x \rangle. \quad (124)$$

Sum over all $p \in \mathcal{B}$, use (21), (23), and (26), and divide by $\sigma \sqrt{2}$ to give

$$0 = \left(\frac{1}{\sqrt{2}} \rho \mathbf{1} - \rho \boldsymbol{\Theta} \right)' + \frac{1}{\sqrt{2}} \sum_{p \in \mathcal{B}} \left\langle m \mathbf{1} (\nabla_{x_p} W \cdot \mathbf{v}_p) \mid x_p = x \right\rangle - \sum_{p \in \mathcal{B}} \left\langle \frac{1}{2} m \mathbf{d}_p \odot \mathbf{d}_p (\nabla_{x_p} W \cdot \mathbf{v}_p) \mid x_p = x \right\rangle + \rho (\dot{\boldsymbol{\Theta}} + \boldsymbol{\Delta}). \quad (125)$$

With an identity involving the divergence and (22), it follows that

$$\sum_{p \in \mathcal{B}} \left\langle m \mathbf{1} (\nabla_{x_p} W \cdot \mathbf{v}_p) \mid x_p = x \right\rangle = \operatorname{div}_x \sum_{p \in \mathcal{B}} \left\langle \mathbf{1} \otimes (m \mathbf{v}_p) W \mid x_p = x \right\rangle = \operatorname{div}_x (\mathbf{1} \otimes \rho \mathbf{v}) = \operatorname{div}_x (\rho \mathbf{v}) \mathbf{1}. \quad (126)$$

Further, in view of the identity

$$\frac{1}{2} (\mathbf{d}_p \odot \mathbf{d}_p) \otimes \mathbf{v}_p = \left(\frac{1}{2} \mathbf{d}_p \odot \mathbf{d}_p - \boldsymbol{\Theta} \right) \otimes (\mathbf{v}_p - \mathbf{v}) + \frac{1}{2} (\mathbf{d}_p \odot \mathbf{d}_p) \otimes \mathbf{v} + \boldsymbol{\Theta} \otimes \mathbf{v}_p - \boldsymbol{\Theta} \otimes \mathbf{v}, \quad (127)$$

the identifications (21)–(24) give

$$\begin{aligned} \sum_{p \in \mathcal{B}} \left\langle \frac{1}{2} m \mathbf{d}_p \odot \mathbf{d}_p (\nabla_{x_p} W \cdot \mathbf{v}_p) \mid x_p = x \right\rangle &= \operatorname{div}_x \sum_{p \in \mathcal{B}} \left\langle \frac{1}{2} m (\mathbf{d}_p \odot \mathbf{d}_p) \otimes \mathbf{v}_p W \mid x_p = x \right\rangle \\ &= \operatorname{div}_x (-\mathbb{I} + \boldsymbol{\Theta} \otimes \rho \mathbf{v}) \\ &= -\operatorname{div}_x \mathbb{I} + \nabla_x \boldsymbol{\Theta} (\rho \mathbf{v}) + \boldsymbol{\Theta} \operatorname{div}_x (\rho \mathbf{v}). \end{aligned} \quad (128)$$

Finally, to obtain the tensor moment of inertia balance (12), use (126) and (128) in (125) and apply the mass balance (11).

5.3 Momentum balance

Let p in $\mathcal{B}$ be given. Multiply (8) by $m \mathbf{v}_p$, integrate over Ω_p , and set $x_p = x$ to obtain

$$0 = \langle m \mathbf{v}_p W' \mid x_p = x \rangle + \sum_{q \in \mathcal{B}} [\langle m \mathbf{v}_p (\nabla_{x_q} W \cdot \mathbf{v}_q) \mid x_p = x \rangle + \langle \mathbf{v}_p \operatorname{div}_{\mathbf{v}_q} (w(-\nabla_{x_q} \psi + \mathbf{f}_q^{\text{ni}})) \mid x_p = x \rangle + \langle m \mathbf{v}_p \nabla_{\mathbf{d}_q} \cdot \mathbf{s}_q \mid x_p = x \rangle + \langle \frac{m}{I} \mathbf{v}_p \mid x_p = x \rangle]$$

(129)

Integrate by parts, dropping all terms that vanish, to leave

$$0 = \langle m \mathbf{v}_p W' \mid x_p = x \rangle + \langle m \mathbf{v}_p (\nabla_{x_p} W \cdot \mathbf{v}_p) \mid x_p = x \rangle + \langle W \nabla_{x_p} \psi \mid x_p = x \rangle - \langle \mathbf{f}_p^{\text{ni}} W \mid x_p = x \rangle.$$

(130)

Since m and $\mathbf{v}_p$ do not depend on x_p , an identity involving the divergence implies that $\operatorname{div}_{x_p} [m(\mathbf{v}_p \otimes \mathbf{v}_p W)] = m \mathbf{v}_p (\nabla_{x_p} W \cdot \mathbf{v}_p)$. Use this identity and sum (130) over all p in $\mathcal{B}$ to give

$$0 = \left(\sum_{p \in \mathcal{B}} \langle m \mathbf{v}_p W \mid x_p = x \rangle \right)' + \operatorname{div}_x \sum_{p \in \mathcal{B}} \langle m \mathbf{v}_p \otimes \mathbf{v}_p W \mid x_p = x \rangle - \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \langle \mathbf{f}_{pq} W \mid x_p = x \rangle - \sum_{p \in \mathcal{B}} \langle \mathbf{f}_p^{\text{ni}} W \mid x_p = x \rangle.$$

(131)

Use the identity

$$\mathbf{v}_p \otimes \mathbf{v}_p = (\mathbf{v}_p - \mathbf{v}) \otimes (\mathbf{v}_p - \mathbf{v}) + \mathbf{v} \otimes \mathbf{v}_p + \mathbf{v}_p \otimes \mathbf{v} - \mathbf{v} \otimes \mathbf{v}, \quad (132)$$

to simplify the second term in (131), which, on invoking the identifications (21)–(29), becomes

$$\operatorname{div}_x (-\mathbf{T}_K + \rho \mathbf{v} \otimes \mathbf{v}). \quad (133)$$

Isolate the third term on the right-hand side of (131), use a lemma due to Pitteri [38] and (30), to give

$$\begin{aligned}
 & - \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \langle \mathbf{f}_{pq} W \mid x_p = x \rangle = - \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_{\mathcal{E}} \langle \mathbf{f}_{pq} W \mid x_p = x, x_q \\
 & = \tilde{x} \rangle d\tilde{x} \\
 & = \frac{1}{2} \operatorname{div}_x \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_{\gamma} \int_0^\infty \langle \mathbf{f}_{pq} W \mid x_p = x + \alpha \mathbf{z}, x_q \\
 & = x - (1 - \alpha) \mathbf{z} \rangle \otimes \mathbf{z} d\alpha \, dz = - \operatorname{div}_x \mathbf{T}_I.
 \end{aligned}$$

Use this equality, (133), and the identifications (22) and (43) in (131) to give

$$0 = (\rho \mathbf{v})' + \operatorname{div}_x (-\mathbf{T} + \rho \mathbf{v} \otimes \mathbf{v}) - \rho \mathbf{b}. \quad (134)$$

Finally, to obtain the linear momentum balance (13), expand the term $\operatorname{div}_x (\rho \mathbf{v} \otimes \mathbf{v})$, apply the mass balance (11), and use the identity $\dot{\mathbf{v}} = \mathbf{v}' + (\nabla \mathbf{v}) \mathbf{v}$.

5.4 Moment of momentum balance

Let p in $\mathcal{B}$ and y in $\mathcal{E}$ be given. Multiply (8) by the moment of momentum $\mathbf{L}_p(y) = m(x_p - y) \wedge \mathbf{v}_p + \mathbf{I}_p \mathbf{s}_p$ of rod p about y , integrate over Ω_p , and set $x_p = x$ to obtain

$$\begin{aligned}
 0 = \langle \mathbf{L}_p(y) W' \mid x_p = x \rangle + \sum_{q \in \mathcal{B}} [\langle \mathbf{L}_p(y) \nabla_{x_q} W \cdot \mathbf{v}_q \mid x_p = x \rangle + \langle \frac{1}{m} \mathbf{L}_p(y) \operatorname{div}_{\mathbf{v}_q} (W (-\nabla_{x_q} \psi + \mathbf{f}_q^{\text{ni}})) \mid x_p = x \rangle + \langle \mathbf{L}_p(y) \nabla_{\mathbf{d}_q} W \cdot \mathbf{s}_q \mid x_p = x \rangle] \\
 \quad (135)
 \end{aligned}$$

Integrate by parts, dropping terms that vanish, to leave

$$\begin{aligned}
 0 = \langle \mathbf{L}_p(y) W' \mid x_p = x \rangle + \langle \mathbf{L}_p(y) \nabla_{x_q} W \cdot \mathbf{v}_q \mid x_p = x \rangle + \langle (x_p - y) \wedge \nabla_{x_p} \psi W \mid x_p = x \rangle - \langle (x_p - y) \wedge \mathbf{f}_p^{\text{ni}} W \mid x_p = x \rangle + \langle \mathbf{d}_p \wedge \nabla_{\mathbf{d}_p} \psi W \mid x_p = x \rangle - \langle \mathbf{d}_p \wedge \mathbf{c}_p^{\text{nl}} W \mid x_p = x \rangle. \quad (136)
 \end{aligned}$$

Sum over all p in $\mathcal{B}$ and use (22) and (25) on the first term, as well as (43) and (44), to give

$$0 = ((x - y) \wedge \rho \mathbf{v} + \rho \sigma \mathbf{S})' + \mathbf{V}_1 + \mathbf{V}_2 - (x - y) \wedge \rho \mathbf{b} - \rho \mathbf{B}, \quad (137)$$

where

$$\mathbf{V}_1 := \sum_{p \in \mathcal{B}} \langle \mathbf{L}_p(y) (\nabla_{x_p} W \cdot \mathbf{v}_p) \mid x_p = x \rangle,$$

$$\mathbf{V}_2 := \sum_{p \in \mathcal{B}} \langle (x_p - y) \wedge \nabla_{x_p} \psi W \mid x_p = x \rangle + \sum_{p \in \mathcal{B}} \langle \mathbf{d}_p \wedge \nabla_{\mathbf{d}_p} \psi W \mid x_p = x \rangle.$$

Use identities involving the divergence to give

$$\mathbf{V}_1 = (x - y) \wedge \operatorname{div}_x \sum_{p \in \mathcal{B}} \langle m \mathbf{v}_p \otimes \mathbf{v}_p W \mid x_p = x \rangle + \operatorname{div}_x \sum_{p \in \mathcal{B}} \langle I(\mathbf{d}_p \wedge \mathbf{s}_p) \otimes \mathbf{v}_p W \mid x_p = x \rangle.$$

(138)

Further, use the identity

$$(\mathbf{d}_p \wedge \mathbf{s}_p) \otimes \mathbf{v}_p = (\mathbf{d}_p \wedge \mathbf{s}_p - \mathbf{S}) \otimes (\mathbf{v}_p - \mathbf{v}) + \mathbf{S} \otimes \mathbf{v}_p (\mathbf{d}_p \wedge \mathbf{s}_p) \otimes \mathbf{v} - \mathbf{S} \otimes \mathbf{v}, \quad (139)$$

the fact that $I = \sigma m$, (21), (22), (25), (32), and the argument leading to (133) to give

$$\mathbf{V}_1 = (x - y) \wedge \operatorname{div}_x (-\mathbf{T}_K + \rho \mathbf{v} \otimes \mathbf{v}) + \operatorname{div}_x (-\mathbf{C}_K + \rho \sigma \mathbf{S} \otimes \mathbf{v}). \quad (140)$$

Next, use the definition of $\mathbf{R}_{pq}(y)$, (9), and (10) to give

$$\mathbf{V}_2 = - \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_{\mathcal{E}} \langle \mathbf{R}_{pq}(y) W \mid x_p = x, x_q = \tilde{x} \rangle d\tilde{x}. \quad (141)$$

A lemma due to Pitteri [38] yields

$$\mathbf{V}_2 = \frac{1}{2} \operatorname{div}_x \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_{\mathcal{V}} \int_0^\infty \langle \mathbf{R}_{pq}(y) W \mid x_p = x + \alpha \mathbf{z}, x_q = x - (1 - \alpha) \mathbf{z} \rangle \otimes \mathbf{z} d\alpha d\mathbf{z}. \quad (142)$$

By the definition of $\mathbf{R}_{pq}(y)$, (33), and (34) to give

$$\mathbf{V}_2 + \operatorname{div}_x (\mathbb{C}_{\text{IF}} + \mathbb{C}_{\text{IC}}) = \frac{1}{2} \operatorname{div}_x \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_{\gamma} \int_0^\infty \langle (x-y) \wedge \mathbf{f}_{pq} W \mid x_p = x + \alpha \mathbf{z}, x_q = x - (1-\alpha) \mathbf{z} \rangle \otimes \mathbf{z} d\alpha d\mathbf{z}.$$

(143)

Notice that, by identities involving the divergence and (30), the right-hand side of (143) is equal to

$$\frac{1}{\sqrt{2}} (\mathbf{T}_I - \mathbf{T}_I^\top) - (x-y) \wedge \operatorname{div}_x \mathbf{T}_I. \quad (144)$$

Put (138) and (143) into (137) and use the symmetry of $\mathbf{T}_K$ with (28) to give

$$0 = (\rho(x-y) \wedge \mathbf{v} + \rho \sigma \mathbf{S})' - (x-y) \wedge (\operatorname{div}_x (\mathbf{T} - \rho \mathbf{v} \otimes \mathbf{v}) + \rho \mathbf{b}) + \frac{1}{\sqrt{2}} (\mathbf{T}_I - \mathbf{T}_I^\top) - \operatorname{div}_x (\mathbb{C} - \rho \sigma \mathbf{S} \otimes \mathbf{v}) - \rho \mathbf{B}.$$

(145)

Finally, to obtain the moment of momentum balance (14), expand the terms $\operatorname{div}_x (\rho \mathbf{v} \otimes \mathbf{v})$ and $\operatorname{div}_x (\rho \sigma \mathbf{S} \otimes \mathbf{v})$, apply both the mass balance (11) and the linear momentum balance (13), and use the identity $\dot{\mathbf{S}} = \mathbf{S}' + (\nabla \mathbf{S}) \mathbf{v}$.

5.5 Orientation balance

Let p in $\mathcal{B}$ be given. Multiply (8) by $\mathbf{Id}_p \odot \mathbf{s}_p$, integrate over $\mathcal{Q}_p$, and set $x_p = x$ to obtain

$$0 = \langle \mathbf{Id}_p \odot \mathbf{s}_p W' \mid x_p = x \rangle + \sum_{q \in \mathcal{B}} \left[\langle \mathbf{Id}_p \odot \mathbf{s}_p (\nabla_{x_p} W \cdot \mathbf{v}_q) \mid x_p = x \rangle + \langle \frac{1}{m} \mathbf{d}_p \odot \mathbf{s}_p \operatorname{div}_{\mathbf{v}_q} (W (-\nabla_{x_q} \psi + \mathbf{f}_q^{\text{ni}})) \mid x_p = x \rangle + \langle \mathbf{Id}_p \odot \mathbf{s}_p \nabla_{\mathbf{d}_q} W \mid x_p = x \rangle \right]$$

(146)

Integrate by parts, dropping terms that vanish, to leave

$$\begin{aligned} 0 = & \langle \mathbf{Id}_p \odot \mathbf{s}_p W' \mid x_p = x \rangle + \langle \mathbf{Id}_p \odot \mathbf{s}_p (\nabla_{x_p} W \cdot \mathbf{v}_p) \mid x_p = x \rangle + \langle \mathbf{Id}_p \odot \mathbf{s}_p (\nabla_{\mathbf{d}_p} W \cdot \mathbf{s}_p) + x_p = x \rangle - \langle \mathbf{d}_p \odot \mathbf{s}_p (\nabla_{s_p} W \cdot \mathbf{P}_p \nabla_{\mathbf{d}_p} \psi) \mid x_p = x \rangle - \langle \mathbf{d}_p \odot (\mathbf{P}_p \mathbf{c}_p^{\text{ni}}) W \mid x_p = x \rangle. \end{aligned} \quad (147)$$

Notice that

$$I \mathbf{d}_p \odot \mathbf{s}_p (\nabla_{x_p} W \cdot \mathbf{v}_p) = \text{div}_{x_p} (I (\mathbf{d}_p \odot \mathbf{s}_p) \otimes \mathbf{v}_p W), \quad (148)$$

integrate by parts, and use (10) to give

$$\langle \mathbf{d}_p \odot \mathbf{s}_p (\nabla_{\mathbf{s}_p} W \cdot \mathbf{P}_p \nabla_{\mathbf{d}_p} \psi) \mid x_p = x \rangle = \sum_{q \in \mathcal{B}_p} \langle \mathbf{d}_p \odot \mathbf{P}_p \mathbf{c}_{pq} W \mid x_p = x \rangle, \quad (149)$$

and integrate by parts again to give

$$\langle I \mathbf{d}_p \odot \mathbf{s}_p (\nabla_{\mathbf{d}_p} W \cdot \mathbf{s}_p) \mid x_p = x \rangle = - \langle I \mathbf{s}_p \odot \mathbf{s}_p W \mid x_p = x \rangle + \langle I |\mathbf{s}_p|^2 \mathbf{d}_p \odot \mathbf{d}_p W \mid x_p = x \rangle. \quad (150)$$

Plug these three relations into (147), integrate by parts, sum over all p in $\mathcal{B}$, and use (26) to give

$$\begin{aligned} 0 &= \sigma (\rho \dot{\Theta} + \rho \Delta)' + \text{div}_x \sum_{p \in \mathcal{B}} \langle I (\mathbf{d}_p \odot \mathbf{s}_p) \otimes \mathbf{v}_p W \mid x_p \\ &= x \rangle - \sum_{p \in \mathcal{B}} \langle I \mathbf{s}_p \odot \mathbf{s}_p W \mid x_p \\ &= x \rangle + \sum_{p \in \mathcal{B}} \langle I |\mathbf{s}_p|^2 \mathbf{d}_p \odot \mathbf{d}_p W \mid x_p \\ &= x \rangle - \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \langle \mathbf{d}_p \odot \mathbf{P}_p \mathbf{c}_{pq} W \mid x_p \\ &= x \rangle - \sum_{p \in \mathcal{B}} \langle \mathbf{d}_p \odot \mathbf{P}_p \mathbf{c}_p^{\text{ni}} W \mid x_p = x \rangle. \end{aligned} \quad (151)$$

Use the identity

$$(\mathbf{d}_p \odot \mathbf{s}_p) \otimes \mathbf{v}_p = (\mathbf{d}_p \odot \mathbf{s}_p - (\dot{\Theta} + \Delta)) \otimes (\mathbf{v}_p - \mathbf{v}) + (\dot{\Theta} + \Delta) \otimes \mathbf{v}_p + (\mathbf{d}_p \odot \mathbf{s}_p) \otimes \mathbf{v} - (\dot{\Theta} + \Delta) \otimes \mathbf{v}, \quad (152)$$

the fact that $I = \sigma m$, (21), (22), (26), (27), (35)–(37), (41), and (45) in (151) to give

$$0 = \sigma (\rho \dot{\Theta} + \rho \Delta)' - \rho \sigma \mathbf{H} - \mathbf{N} + \text{div}_x (-\mathbb{L} + \rho \sigma (\dot{\Theta} + \Delta) \otimes \mathbf{v}) - \rho M. \quad (153)$$

Finally, to obtain the orientation balance (15), expand various terms involving the divergence, apply the mass balance (11), and use the identities $\dot{\mathbf{\Theta}} = \mathbf{\Theta}' + (\nabla \cdot \mathbf{\Theta})\mathbf{v}$ and $\dot{\mathbf{v}} = \mathbf{v}' + (\nabla \cdot \mathbf{v})\mathbf{v}$.

5.6 Mesofluctuation balance

Let p in $\mathcal{B}$ be given. Multiply (8) by $\mathbf{I}\mathbf{s}_p \odot \mathbf{s}_p$ integrate over Ω_p and set $x_p = x$ to obtain

$$\begin{aligned} 0 = & \langle \mathbf{I}\mathbf{s}_p \odot \mathbf{s}_p W' \mid x_p \rangle \\ = & \langle x \rangle + \sum_{q \in \mathcal{B}} [\langle \mathbf{I}\mathbf{s}_p \odot \mathbf{s}_p (\nabla_{x_p} W \cdot \mathbf{v}_q) \mid x_p = x \rangle + \langle \frac{I}{m} \mathbf{s}_p \odot \mathbf{s}_p \operatorname{div}_{\mathbf{v}_q} (W (-\nabla_{x_q} \psi + \mathbf{f}_q^{\text{ni}})) \mid x_p = x \rangle + \langle \mathbf{I}\mathbf{s}_p \odot \mathbf{s}_p \nabla_{\mathbf{d}_q} W \cdot \mathbf{s}_q \mid x_p = x \rangle + \langle \mathbf{I}\mathbf{s}_p \odot \mathbf{s}_p \nabla_{\mathbf{d}_q} W \cdot \mathbf{v}_q \mid x_p = x \rangle] \end{aligned} \quad (154)$$

Integrate by parts, dropping terms that vanish, to leave

$$\begin{aligned} 0 = & \langle \mathbf{I}\mathbf{s}_p \odot \mathbf{s}_p W \mid x_p = x \rangle' + \langle \mathbf{I}\mathbf{s}_p \odot \mathbf{s}_p (\nabla_{x_p} W \cdot \mathbf{v}_p) \mid x_p = x \rangle + \langle I |\mathbf{s}_p|^2 \mathbf{s}_p \odot \mathbf{d}_p W \mid x_p = x \rangle + \langle 2\mathbf{s}_p \odot \mathbf{P}_p \nabla_{\mathbf{d}_p} \psi W \mid x_p = x \rangle - \langle 2\mathbf{s}_p \odot \mathbf{P}_p \mathbf{c}_p^{\text{ni}} W \mid x_p = x \rangle. \end{aligned} \quad (155)$$

Use the identity

$$\mathbf{I}\mathbf{s}_p \odot \mathbf{s}_p (\nabla_{x_p} W \cdot \mathbf{v}_p) = \operatorname{div}_{x_p} (I(\mathbf{s}_p \odot \mathbf{s}_p) \otimes \mathbf{v}_p W),$$

(10), sum (155) over all p in $\mathcal{B}$, and invoke the identifications (27) and (46) to give

$$0 = \sigma(\rho \mathbf{H})' + \operatorname{div}_x \sum_{p \in \mathcal{B}} \langle I(\mathbf{s}_p \odot \mathbf{s}_p) \otimes \mathbf{v}_p W \mid x_p = x \rangle - \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \langle 2\mathbf{s}_p \odot \mathbf{P}_p \mathbf{c}_{pq} W \mid x_p = x \rangle - \rho \mathbf{J}. \quad (156)$$

Notice that

$$(\mathbf{s}_p \odot \mathbf{s}_p) \otimes \mathbf{v}_p = (\mathbf{s}_p \odot \mathbf{s}_p - \mathbf{H}) \otimes (\mathbf{v}_p - \mathbf{v}) + \mathbf{H} \otimes \mathbf{v}_p = (\mathbf{s}_p \odot \mathbf{s}_p) \otimes \mathbf{v} - \mathbf{H} \otimes \mathbf{v}. \quad (157)$$

Use this, the fact that $I = \sigma m$, (21), (22), (27), (38)–(40), (42), and (157) in (156) to give

$$0 = \sigma(\rho \mathbf{H})' - Z + \operatorname{div}_x (-\mathbb{G} + \rho \sigma \mathbf{H} \otimes \mathbf{v}) - \rho J. \quad (158)$$

Finally, to obtain the mesofluctuation balance (16), expand various terms involving the divergence, apply the mass balance (11), and use the identity $\dot{\mathbf{H}} = \mathbf{H}' + (\nabla \mathbf{H})\mathbf{v}$.

5.7 Energy balance

Let a rod p in $\mathcal{B}$ be given. Denote by $E_p := k_p + \psi_p$ the energy of the rod p , the kinetic and interaction energies k_p and ψ_p of rod p are as defined by $m|\mathbf{v}_p|^2/2 + I|\mathbf{s}_p|^2/2$ and (97), respectively. Multiply (8) by E_p , integrate over Ω_p , and set $x_p = x$ to obtain

$$\begin{aligned} 0 = & \langle E_p W' \mid x_p = x \rangle + \sum_{q \in \mathcal{B}} [\langle E_p (\nabla_{x_q} W \cdot \mathbf{v}_q) \mid x_p = x \rangle \\ & + \langle \frac{1}{m} E_p \operatorname{div}_{\mathbf{v}_q} (W (-\nabla_{x_q} \psi + \mathbf{f}_q^{\text{ni}})) \mid x_p = x \rangle \\ & + \langle E_p \nabla_{\mathbf{d}_q} W \cdot \mathbf{s}_q \mid x_p = x \rangle + \langle \frac{1}{I} E_p \operatorname{div}_{\mathbf{s}_q} (W \mathbf{P}_q (-\nabla_{\mathbf{d}_q} \psi + \mathbf{c}_q^{\text{ni}})) \mid x_p = x \rangle]. \end{aligned}$$

Integrate by parts, dropping terms that vanish, to leave

$$\begin{aligned} 0 = & \langle E_p W' \mid x_p = x \rangle + \langle E_p (\nabla_{x_q} W \cdot \mathbf{v}_q) \mid x_p = x \rangle \\ & + \sum_{q \in \mathcal{B}} \langle \psi_p (\nabla_{x_q} W \cdot \mathbf{v}_q) \mid x_p = x \rangle \\ & - \langle \frac{1}{m} k_p (\nabla_{\mathbf{v}_p} W \cdot \nabla_{x_p} \psi) \mid x_p = x \rangle \\ & + \sum_{q \in \mathcal{B}} \langle \frac{1}{m} E_p \operatorname{div}_{\mathbf{v}_q} (W \mathbf{f}_q^{\text{ni}}) \mid x_p = x \rangle \\ & + \sum_{q \in \mathcal{B}} \langle \psi_p (\nabla_{\mathbf{d}_q} W \cdot \mathbf{s}_q) \mid x_p = x \rangle - \langle \frac{1}{I} k_p (\nabla_{\mathbf{s}_p} W \cdot \mathbf{P}_p \nabla_{\mathbf{d}_p} \psi) \mid x_p = x \rangle \\ & + \sum_{q \in \mathcal{B}} \langle \frac{1}{I} E_p \operatorname{div}_{\mathbf{s}_q} (W \mathbf{P}_q \mathbf{c}_q^{\text{ni}}) \mid x_p = x \rangle. \end{aligned} \tag{159}$$

Sum over all p in $\mathcal{B}$, integrate by parts, use (47)–(49), (112), and (113) to give

$$0 = \hat{\mathbf{a}} \dot{\mathbf{D}} \mathbf{r}' + \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + \alpha_5 - \rho \mathbf{b} \cdot \mathbf{v} - \rho \mathbf{M} \cdot (\dot{\boldsymbol{\Theta}} + \boldsymbol{\Delta}) - r, \tag{160}$$

where

$$\alpha_1 = \sum_{p \in \mathcal{B}} \langle k_p (\nabla_{x_p} W \cdot \mathbf{v}_p) \mid x_p = x \rangle,$$

$$\alpha_2 = \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}} \langle \psi_p (\nabla_{x_q} W \cdot \mathbf{v}_q) \mid x_p = x \rangle,$$

$$\alpha_3 = \sum_{p \in \mathcal{B}} \langle (\mathbf{v}_p \cdot \nabla_{x_p} \psi) W \mid x_p = x \rangle,$$

$$\alpha_4 = \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}} \langle \psi_p (\nabla_{\mathbf{d}_q} W \cdot \mathbf{s}_q) \mid x_p = x \rangle,$$

$$\alpha_5 = \sum_{p \in \mathcal{B}} \langle (\mathbf{s}_p \cdot \nabla_{\mathbf{d}_p} \psi) W \mid x_p = x \rangle.$$

Use an identity involving the divergence to give

$$\alpha_1 = \operatorname{div}_x \sum_{p \in \mathcal{B}} \langle \left(\frac{1}{2} m |\mathbf{v}_p|^2 \mathbf{v}_p + \frac{1}{2} I |\mathbf{s}_p|^2 \mathbf{v}_p \right) W \mid x_p = x \rangle. \quad (161)$$

Notice that

$$|\mathbf{v}_p|^2 \mathbf{v}_p = |\mathbf{v}_p - \mathbf{v}|^2 (\mathbf{v}_p - \mathbf{v}) + 2[(\mathbf{v}_p - \mathbf{v}) \otimes (\mathbf{v}_p - \mathbf{v})]^\top \mathbf{v} + |\mathbf{v}_p|^2 \mathbf{v} + |\mathbf{v}|^2 (\mathbf{v}_p - \mathbf{v})$$

and

$$|\mathbf{s}_p|^2 \mathbf{v}_p = \left| \mathbf{d}_p \odot \mathbf{s}_p - \dot{\mathbf{\Theta}} - \Delta \right|^2 (\mathbf{v}_p - \mathbf{v}) + 2[(\mathbf{d}_p \odot \mathbf{s}_p - \dot{\mathbf{\Theta}} - \Delta) \otimes (\mathbf{v}_p - \mathbf{v})]^\top (\dot{\mathbf{\Theta}} + \Delta) + |\mathbf{s}_p|^2 \mathbf{v} + \left| \dot{\mathbf{\Theta}} + \Delta \right|^2 (\mathbf{v}_p - \mathbf{v}).$$

Put these into (161) and use (21), (29), (48), (51), and (52) to give

$$\alpha_1 = \operatorname{div}_x \left(\mathbf{q}_{K\mathbf{v}} + q_{K\mathbf{s}} - \mathbf{T}_K^\top \mathbf{v} - \mathbb{L}_K^\top (\dot{\mathbf{\Theta}} + \Delta) + e_K \mathbf{v} \right). \quad (162)$$

Notice that, since both ψ_{pq} and W depend on x_p but $\mathbf{v}_p$ does not, an identity involving the divergence gives

$$\operatorname{div}_{x_p} (\psi_{pq} \mathbf{v}_p W) = \mathbf{v}_p \cdot \nabla_{x_p} \psi_{pq} W + \psi_{pq} \mathbf{v}_p \cdot \nabla_{x_p} W. \quad (163)$$

Consider a_2 . By the definition of ψ_p (97), (163)

$$\begin{aligned}\alpha_2 = & \sum_{p \in \mathcal{B}} \langle \psi_p (\nabla_{x_p} W \\ & \cdot \mathbf{v}_p) \mid x_p = x \rangle + \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \langle \psi_p (\nabla_{x_q} W \cdot \mathbf{v}_q) \mid x_p = x \rangle = \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \langle \frac{1}{2} \psi_{pq} (\nabla_{x_p} W \\ & \cdot \mathbf{v}_p) \mid x_p = x \rangle + \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \sum_{r \in \mathcal{B}_p} \langle \frac{1}{2} \psi_{pr} (\nabla_{x_q} W \cdot \mathbf{v}_p) \mid x_p = x \rangle = \frac{1}{2} \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} (\operatorname{div}_x \langle \psi_{pq} \mathbf{v}_p W \mid x_p = x \rangle + \langle \mathbf{f}_{pq} \cdot \mathbf{v}_p W \mid x_p = x \rangle)\end{aligned}$$

Since $a_3 = - \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \langle \mathbf{f}_{pq} \cdot \mathbf{v}_p W \mid x_p = x \rangle$, it follows from $\mathbf{f}_{pq} = -\mathbf{f}_{qp}$ that

$$\alpha_2 + \alpha_3 = \frac{1}{2} \operatorname{div}_x \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \langle \psi_{pq} \mathbf{v}_p W \mid x_p = x \rangle - \frac{1}{2} \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \langle \mathbf{f}_{pq} \cdot (\mathbf{v}_p + \mathbf{v}_q) W \mid x_p = x \rangle. \quad (164)$$

Use (53) and (49), to obtain

$$\frac{1}{2} \operatorname{div}_x \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \langle \psi_{pq} \mathbf{v}_p W \mid x_p = x \rangle = \operatorname{div}_x (\mathbf{q}_T + \hat{\mathbf{a}} \tilde{\mathbf{D}} \mathbf{f}_I \mathbf{v}). \quad (165)$$

Use a lemma due to Pitteri [38], (30), and (54) to give

$$\begin{aligned}& - \frac{1}{2} \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \langle \mathbf{f}_{pq} \\ & \cdot (\mathbf{v}_p + \mathbf{v}_q) W \mid x_p = x \rangle = - \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_{\mathcal{E}} \langle \mathbf{f}_{pq} \\ & \cdot (\frac{\mathbf{v}_p + \mathbf{v}_q}{2}) W \mid x_p = x, x_q \\ & = \tilde{x} \rangle d\tilde{x} \\ & = \operatorname{div}_x \frac{1}{2} \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_v \int_0^\infty \langle [\mathbf{f}_{pq} \cdot (\frac{\mathbf{v}_p + \mathbf{v}_q}{2})] z W \mid x_p = x + \alpha \mathbf{z}, x_q \\ & = x - (1 - \alpha) \mathbf{z} \rangle d\alpha d\mathbf{z} \quad (166)\end{aligned}$$

$$= \operatorname{div}_x (\mathbf{q}_{\text{If}} - \mathbf{T}_I^\top \mathbf{v}). \quad (167)$$

Put (165) together with (167), finding that

$$\alpha_2 + \alpha_3 = \operatorname{div}_x (\mathbf{q}_T + \mathbf{q}_{\text{If}} - \mathbf{T}_I^\top \mathbf{v} + e_I \mathbf{v}). \quad (168)$$

Consider a_4 , use the definition of ψ_p (97), and integrate by parts to give

$$\alpha_4 = \frac{1}{2} \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} (\langle \mathbf{c}_{pq} \cdot \mathbf{s}_p W \mid x_p = x \rangle + \langle \mathbf{c}_{qp} \cdot \mathbf{s}_q W \mid x_p = x \rangle). \quad (169)$$

Since $\alpha_5 = - \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \langle \mathbf{c}_{pq} \cdot \mathbf{s}_p W \mid x_p = x \rangle$,

$$\alpha_4 + \alpha_5 = \frac{1}{2} \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \langle (\mathbf{c}_{pq} \cdot \mathbf{s}_p - \mathbf{c}_{qp} \cdot \mathbf{s}_q) W \mid x_p = x \rangle. \quad (170)$$

Use a lemma due to Pitteri [38], (37), and (55), to give

$$\begin{aligned} \alpha_4 + \alpha_5 &= - \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_{\mathcal{E}} \langle \frac{1}{2} (\mathbf{c}_{pq} \\ &\quad \cdot \mathbf{s}_p - \mathbf{c}_{qp} \cdot \mathbf{s}_q) W \mid x_p = x, x_q \\ &= \tilde{x} \rangle d\tilde{x} \\ &= \operatorname{div}_x \frac{1}{2} \sum_{p \in \mathcal{B}} \sum_{q \in \mathcal{B}_p} \int_v \int_0^\infty \langle \frac{1}{2} (\mathbf{c}_{pq} \\ &\quad \cdot \mathbf{s}_p - \mathbf{c}_{qp} \cdot \mathbf{s}_q) \mathbf{z} W \mid x_p = x + \alpha \mathbf{z}, x_q \\ &= x - (1 - \alpha) \mathbf{z} \rangle d\alpha d\mathbf{z} \\ &= \operatorname{div}_x (\mathbf{q}_{\text{IC}} \\ &\quad - \mathbb{L}_1^\top (\dot{\boldsymbol{\Theta}} + \boldsymbol{\Delta})). \end{aligned} \quad (171)$$

Finally, to obtain the energy balance (17), combine (28), (35), (50), (160), (162), (168), (171), and use the identity $e' + \operatorname{div}(\mathbf{e}\mathbf{v}) = e + \operatorname{div} \mathbf{v}$.

6 Summary

A statistical derivation of the macroscopic balance laws (11)–(17) for liquid crystals—with microstructure described by a symmetric and traceless tensor—was provided. The derivation begins with a microscopic model consisting of a discrete system of rigid rods. The statistical approach rests on the introduction of a probability density W consistent with the principle of conservation of probability and, thus, satisfying a Liouville equation. This evolution equation serves as the starting point for the derivation of the macroscopic balance laws. The general procedure for obtaining a macroscopic balance law from the Liouville equation is outlined at the outset of Section 5.

The macroscopic balance laws (11)–(17) emerge on interpreting the terms that comprise them as expected values. Statistical formulas for these terms are justified in

Section 4. These balances were compared 26 with the balances of MacMillian [23] and conditions under what assumptions the balances (11)–(17) reduce to those of MacMillian [23] were provided. The primary difference between the balance laws obtained in the present work and those of MacMillian [23] resides in the orientation balance. The orientation balance (15) derived in the present work contains two additional terms, both of which are inertial in nature and have clear discrete interpretations. One of these, which involves the relative average rate, appears in the work of Pitteri [4]. The other, which involves the Reynolds tensor, appears in the works of Capriz [30] and Capriz & Brocato [31]. Consistent with their inertial character, the relative average rate and the Reynolds tensor are regulated by additional balance laws: whereas the relative average rate is determined by the orientation flux tensor through (12), the Reynolds tensor is governed by the mesofluctuation balance (16). It should be noted that Capriz's [30] theory of ephemeral continua also has a tensor moment of inertial balance but the form of this balance is very different from (12).

It is possible that the additional terms in the orientation balance (15) might be negligible under many, if not all, circumstances. However, to investigate the relevance of these relative average rate and the Reynolds tensor to the evolution of a liquid crystal, it would be necessary to introduce constitutive relations, boundary conditions, and initial conditions, closing the system of partial differential equations. To ensure consistency of the constitutive relations with thermodynamics, it would first be necessary to derive or postulate a statement of the second law of thermodynamics. Such a task is beyond the scope of this work and is therefore left for future investigations. At the very least, in situations where the additional terms are not essential, our developments provide a microscopic basis for the equations of MacMillan [23].

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